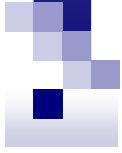


Computational physics and chemistry with ABINIT


SC 2009 - Portland

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OUTLINE

- **Brief Introduction**
- **What is ABINIT**
- **Running ABINIT**
- **Sample runs**



Computational
chemistry/physics/material science
Packages (\$\$\$)

- Gaussian 09
- Crystal
- CASTEP
- Wien 2k
- VASP
- Molpro
- ...




Computational chem/phys/materials science Software (**Free**)

- Gamess
- Nwchem
- Mopac
- QMC
- **ABINIT**
- ...

See:

<http://www.redbrick.dcu.ie/~noel/linux4chemistry/>



ABINIT (=AB-INITio†)

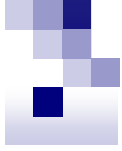
ABINIT is an

- Open-source (OK to distribute, modify, etc.)
- Free (no license)
- Portable (Linux, Windows, Mac)

computational chemistry/physics/materials science package

- (1) Plane-wave-based ($\sim e^{kx}$)
- (2) Pseudopotential
- (3) Density Functional Theory-based (DFT)

† First-principles (from the beginning)



ABINIT (www.abinit.org)

(1) **Plane-wave** (real-space \rightarrow k-space \rightarrow real-space) †††

(2) **Pseudopotential instead of “full” electron calculations** †

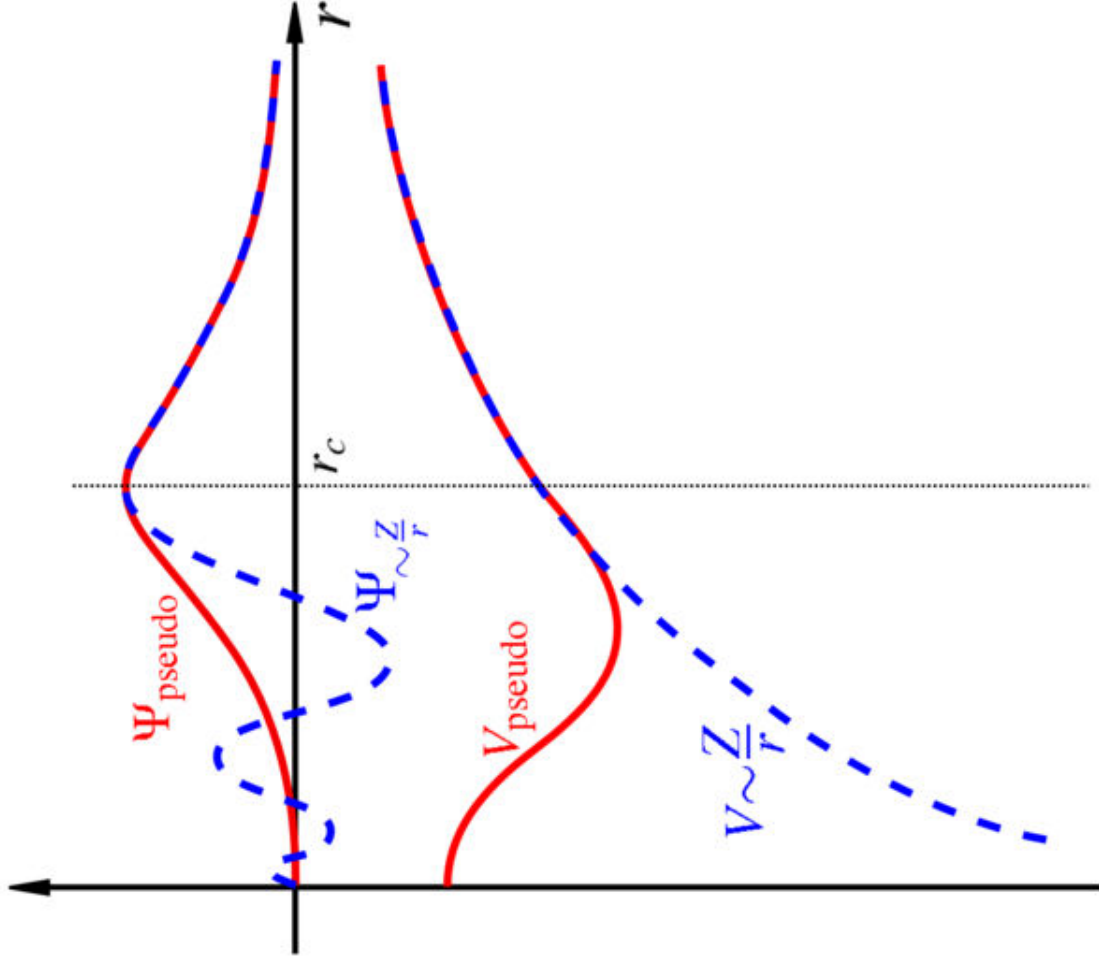
††† = Expensive

† = Cheap, if you know how to do it

Pseudopotential

“All” electron calculation
> very, very expensive
and complicated

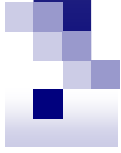
Replace with
“pseudopotential”





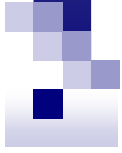
What can ABINIT do?

- Total energy calculations
- Band/electronic structure calculations
 - Electron/charge density
 - Eigenvalues
 - Density of States
- Structural optimizations
- Magnetic structure (with spin) calculations
- Molecular dynamics
- Excited state calculations (via TDDFT & GW /many body approximation)
- Corrections (GGA/LDA + U, Projected Augmented Wave)
- Etc....

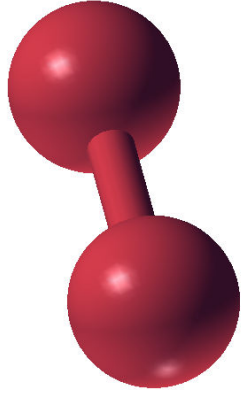


What structures can be calculated?

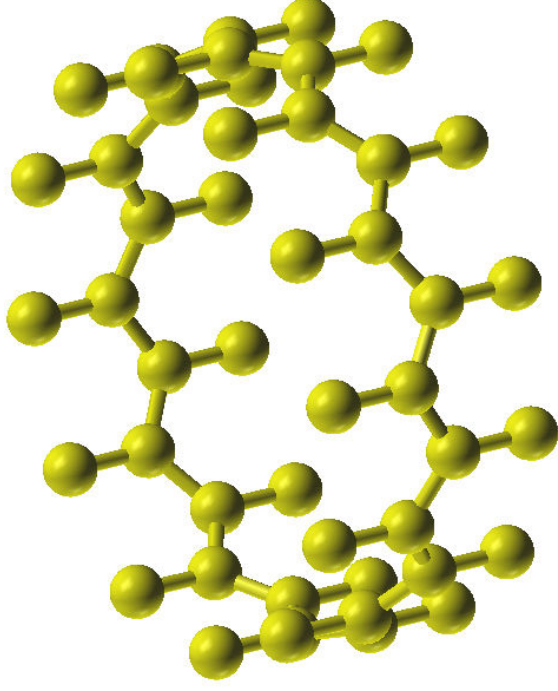
1. Isolated atoms/clusters
2. Periodic structures (solid state structures)



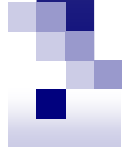
Structures



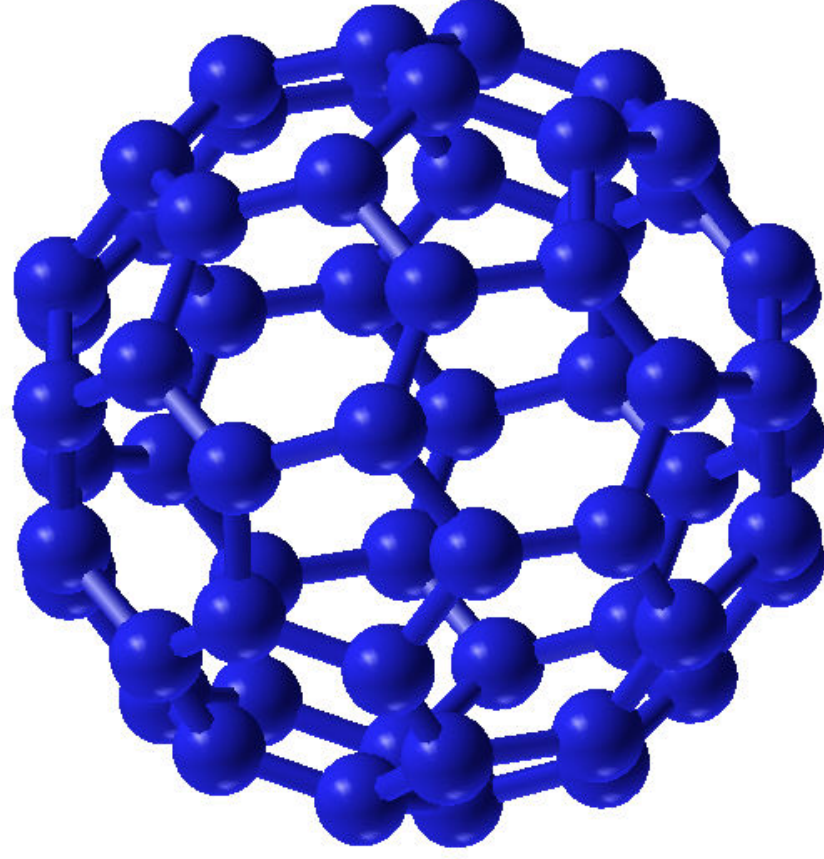
Hydrogen (H_2)



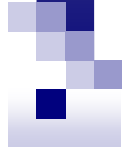
Carbon NanoRing



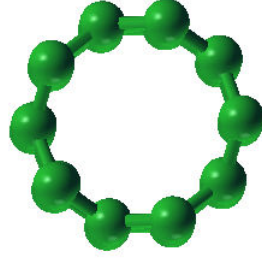
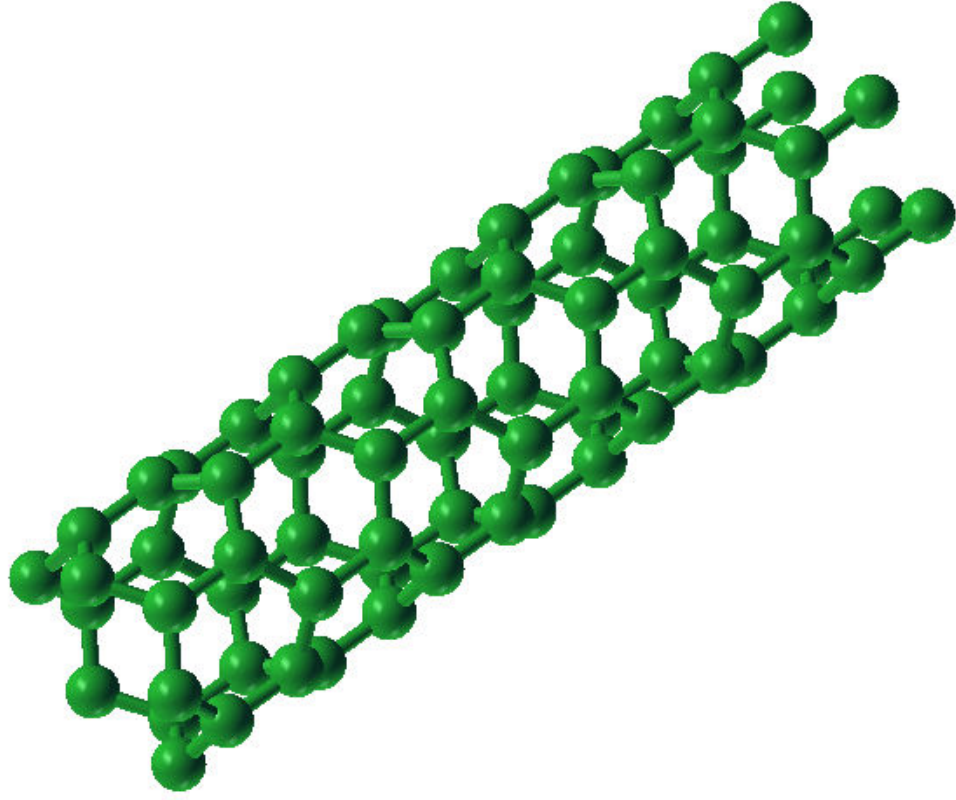
Structures

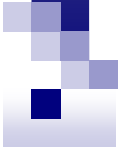


C60 Buckyball

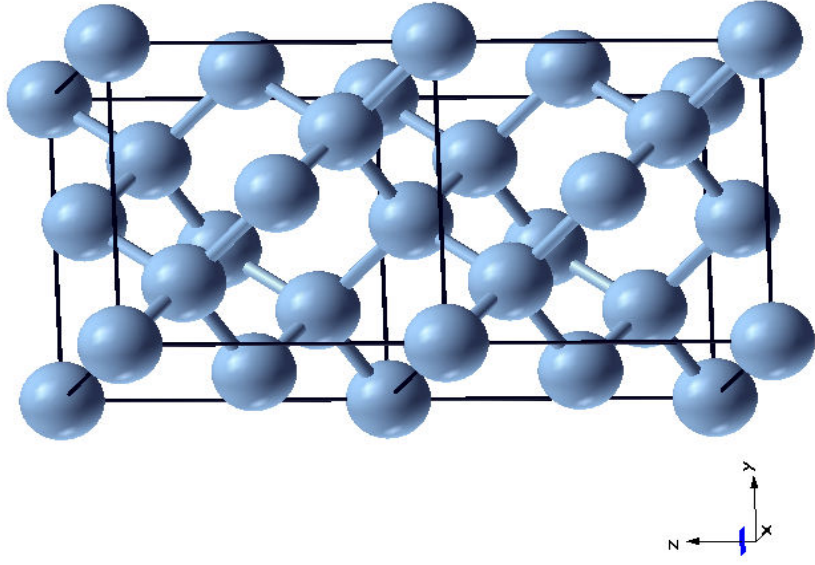


Structures

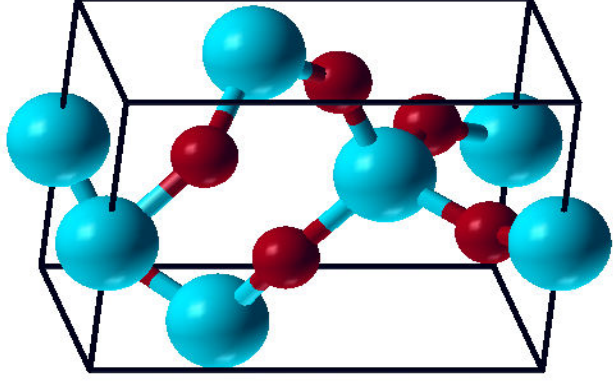




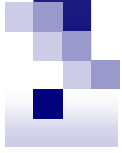
Structures



Silicon



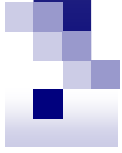
Quartz



ABINIT parallelization

YES !!! (through MPI)

- k-point parallelization (the easiest)
- Band parallelization
- Spin parallelization
- FFT parallelization (grid)
- Benchmarking (??)



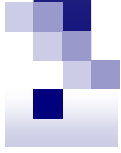
Running ABINIT

INPUT files (needed!):

- ABINIT binary (abinip or abinis)
- Input file (*.in)
- Files file (*.files)
- Pseudopotential file

OUTPUT files:

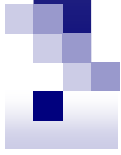
- *.out
- *.log
- Several other files



Preparing input file

Key input file: *.in

- Specify the structure: Unit cell, the initial position of each atom, etc.
- Specify the atom(s): Types, how many, etc.
- Specify the basis set
- Specify the k-point grid
- Specify the convergence procedure



Preparing input file

Some basic input parameters:

acell x y z # Primitive vectors (Bohr)

ntypat # type of atom

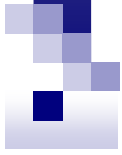
znucl # atomic number of atom

natom # number of atom

typat # type of atom

xcart # Cartesian coordinate

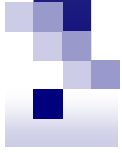
xred # Reduced coordinate



Preparing input file

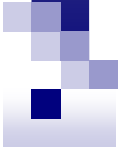
Some basic input parameters:

```
ecut # Pseudopotential energy cut
nkpt # Number of k-point (expensive)
nstep # Maximal number of SCF cycles
toldfe # Tolerance
etc... etc...
```



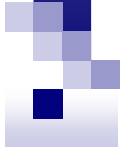
How long does a calculation take?

It depends (How much time do you want to wait, How big is your system? How accurate? Etc..)



“Small” calculations

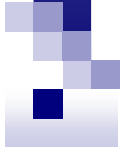




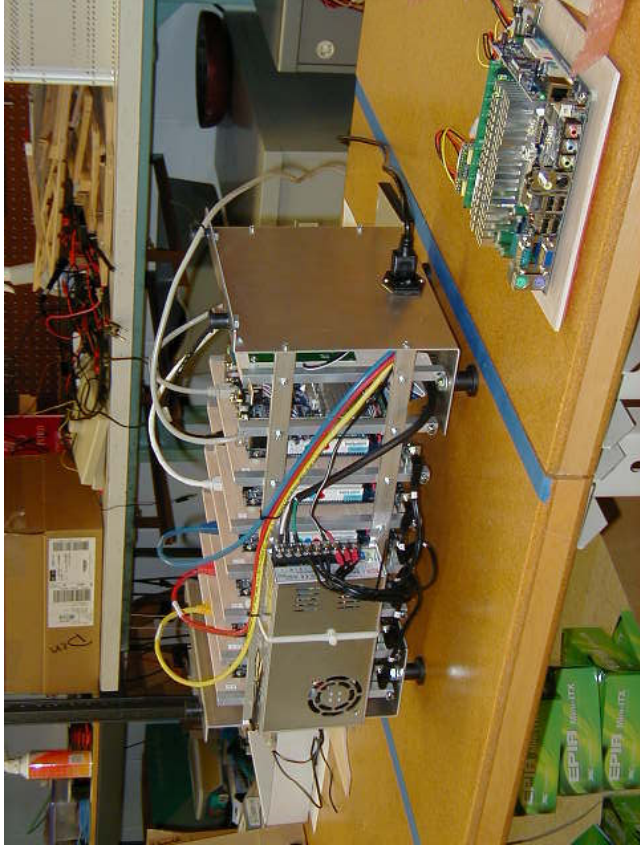
“Big” calculations



IBM “Roadrunner” (#1 TOP500 6/09)



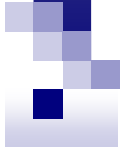
LittleFe (www.littlefe.net)



A “small” cluster with “big” capability
Courtesy of Northern Iowa University
Earlham College



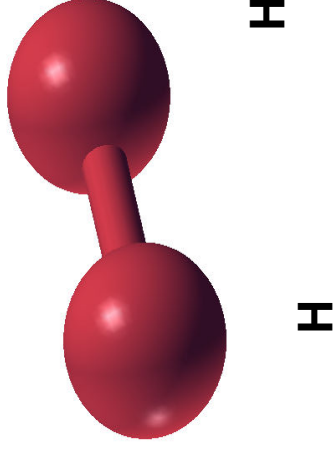
Let's run some cases




```
* ssh to chi.kean.edu using  
putty
```

```
* Login  
* ssh puma
```

Example 1 (H_2)




- Place 2 Hydrogen atoms in a “large” cube space (a cell of size $10 \times 10 \times 10$ a.u.) Set distance = 1.4 Bohr



Example 1 (H₂)

- cd to abinit-sc09 directory (cd abinit-sc09)
- Look at the h2a.in file
- Look at the h2a.files file
- Look at the 01h.pspgth (pseudopotential)
- Run ABINIS (must use full path)

```
/share/apps/bin/abinis < h2a.files >& h2a.log
```



Example 1 (H₂)

- Several output files
- Look briefly at h2a.log
- Look closely at h2a.out (energy)

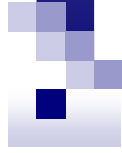


Example 2 (H₂ optimization)

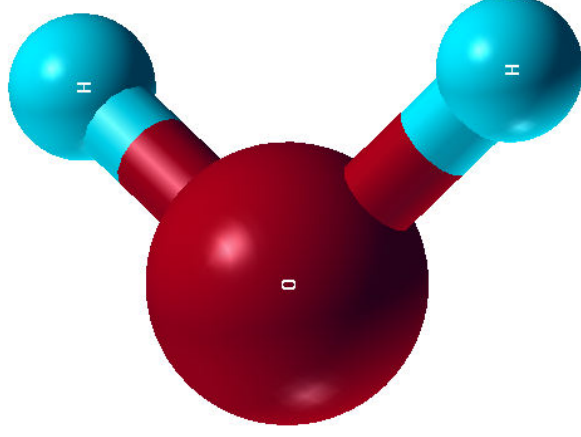
- Look at h2b.in file
 - ionmov ≠ 0
- Run ABINIS

```
/share/apps/bin/abinis < h2b.files >& h2b.log
```

- Done ...
- Look at the h2b.out file, especially the position of the atoms (~ 1.47 Bohr compared to 1.401 Bohr exp.)



Example 3 (H₂O optimization)



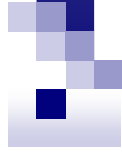


Example 3 (H₂O optimization)

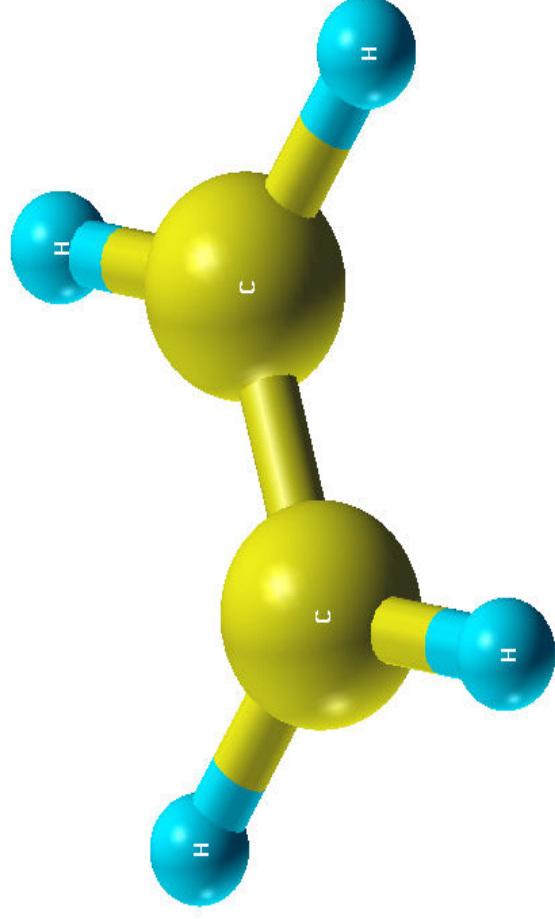
- Look at h2o-opt.in file
 - ionmov ≠ 0
- Run ABINIS

```
/share/apps/bin/abinis < h2o-opt.files >&  
h2o-opt.log
```

- Done ...
- Look at the h2o-opt.out file, especially the position of the atoms (H₂O)



Example 4 (C_2H_4 optimization)



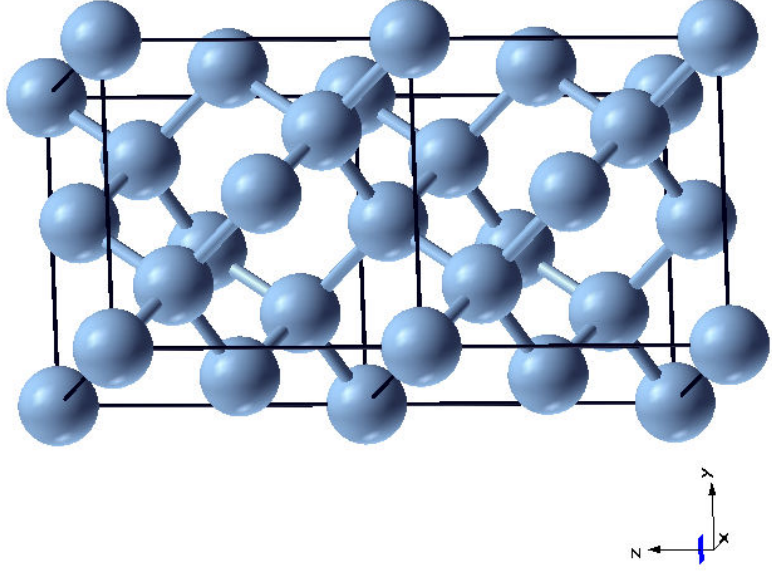
Example 4 (C₂H₄ optimization)

- Look at c2h4.in file
 - ionmov ≠ 0
- Run ABINIS

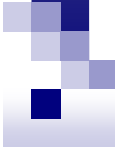
```
/share/apps/bin/abinis < c2h4.files >&  
c2h4.log
```

- Done ...
- Look at the c2h4.out file, especially the position of the atoms

Example 5 (Silicon)



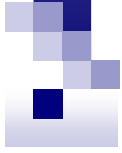
- Place 2 Silicon atoms in the “primitive” cell



Example 5 (Silicon)

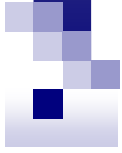
- Assuming you're still in abinit library
- Look at the si.in file (especially ecut)
- Look at the si.files file
- Look at the si pseudopotential
- Run ABINIS

```
/share/apps/bin/abinit < si.files >& si.log
```



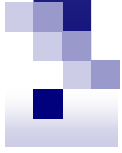
Example 5 (Silicon)

- Several output files
- Look briefly at si.log
- Look closely at si.out (energy)



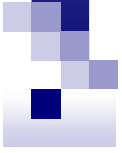
Example 6 (Silicon – Lattice constant optimization)

- Redo example 5
- Lattice constant has changed

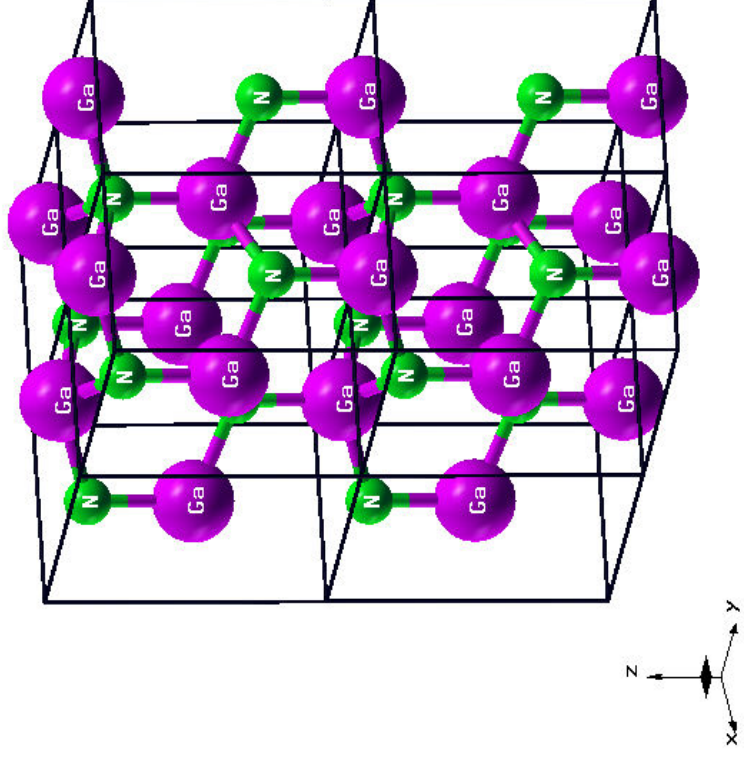



Example 7 (Silicon – Band Structure)

- Redo example 5
- Band structure (0,0,0 = Gamma point)



Example 8 (GaN crystal)

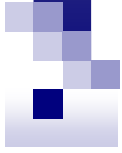




Example 8 (GaN)

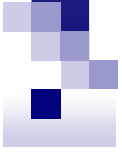
- Look at the gan.in file (especially ecut)
- Look at the gan.files file
- Look at the gan.psp
- Run ABINIS

```
/share/apps/bin/abinis < gan.files >&  
gan.log
```

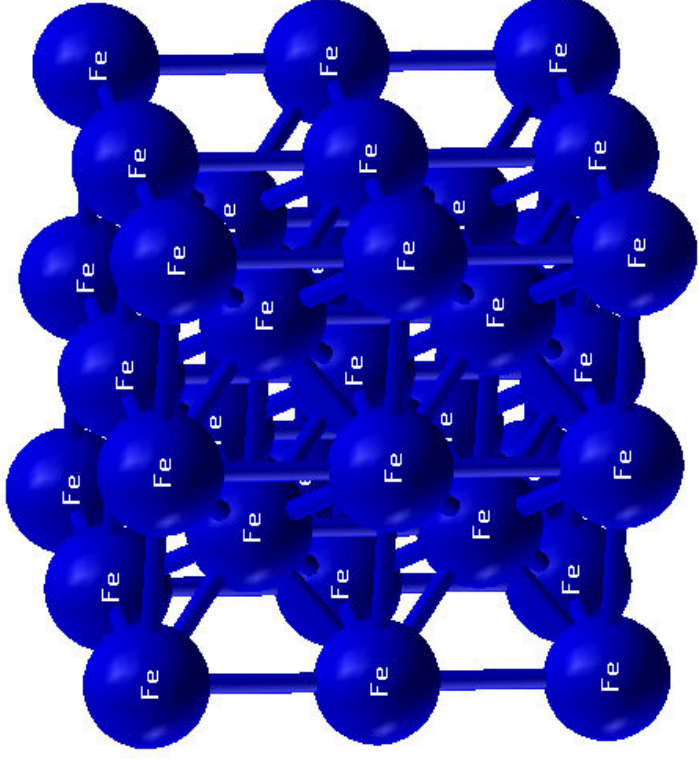


Example 8 (GAN)

- Look briefly at the `gan.log` file
- Look closely at the `gan.out` (energy)



Example 9 (Iron)

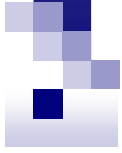




Example 9 (Ferromagnetic Iron)

- Look at the fe.in file (especially ecut)
- Look at the fe.files file
- Look at the fe.psp
- Run ABINIS

```
/share/apps/bin/abinis < fe.files >& fe.log
```



Example 9 (Ferromagnetic Iron)

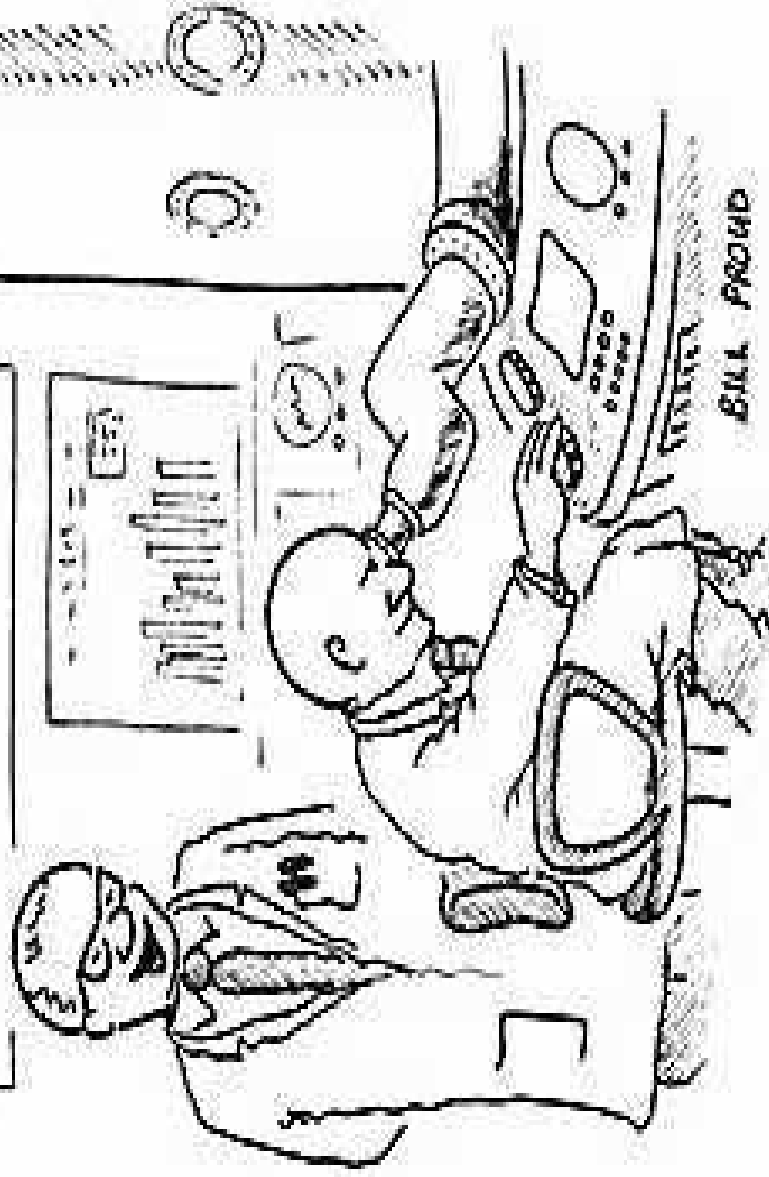
- Look briefly at the fe.log file
- Look closely at the fe.out file
(magnetization)

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NANOTECHNOLOGY



"If you increase the magnification another million times you can see the safety regulations."

"Perhaps I overdid the nano
and underdid the bio!"

