# Example 1

## Bulk silicon

# Instructions (I)

- Have a look at the input file (silicon.fdf)
- Run siesta:

```
siesta < silicon.fdf | tee silicon.out
```

- Check output file (silicon.out):
  - System type
  - Mesh cutoff
  - SCF steps
  - Forces & stress tensor
- Find eigen-energies file (silicon.EIG)

# silicon.fdf

```
SystemName          silicon
SystemLabel         silicon
NumberOfAtoms       2
NumberOfSpecies     1

%block ChemicalSpeciesLabel
 1  14  Si
%endblock ChemicalSpeciesLabel

LatticeConstant     5.430 Ang

%block LatticeVectors
  0.500  0.500  0.000
  0.500  0.000  0.500
  0.000  0.500  0.500
%endblock LatticeVectors

AtomicCoordinatesFormat   ScaledCartesian

%block AtomicCoordinatesAndAtomicSpecies
  0.000   0.000   0.000    1   Si
  0.250   0.250   0.250    1   Si
%endblock AtomicCoordinatesAndAtomicSpecies
```

# Instructions (II)

- Check silicon.long.fdf
- Run silicon.long.fdf :

```
siesta < silicon.long.fdf | tee silicon.out
```

- Plot band structure.
  - Use gnubands

```
gnubands <silicon.bands | tee bands,dat
```

  - Plot bands.dat
    - xmgrace bands.dat &
    - Select correct range of energies

# SUMMER SCHOOL ON COMPUTATIONAL MATERIALS SCIENCE

## University of Illinois at Urbana-Champaign, June 13-23, 2005

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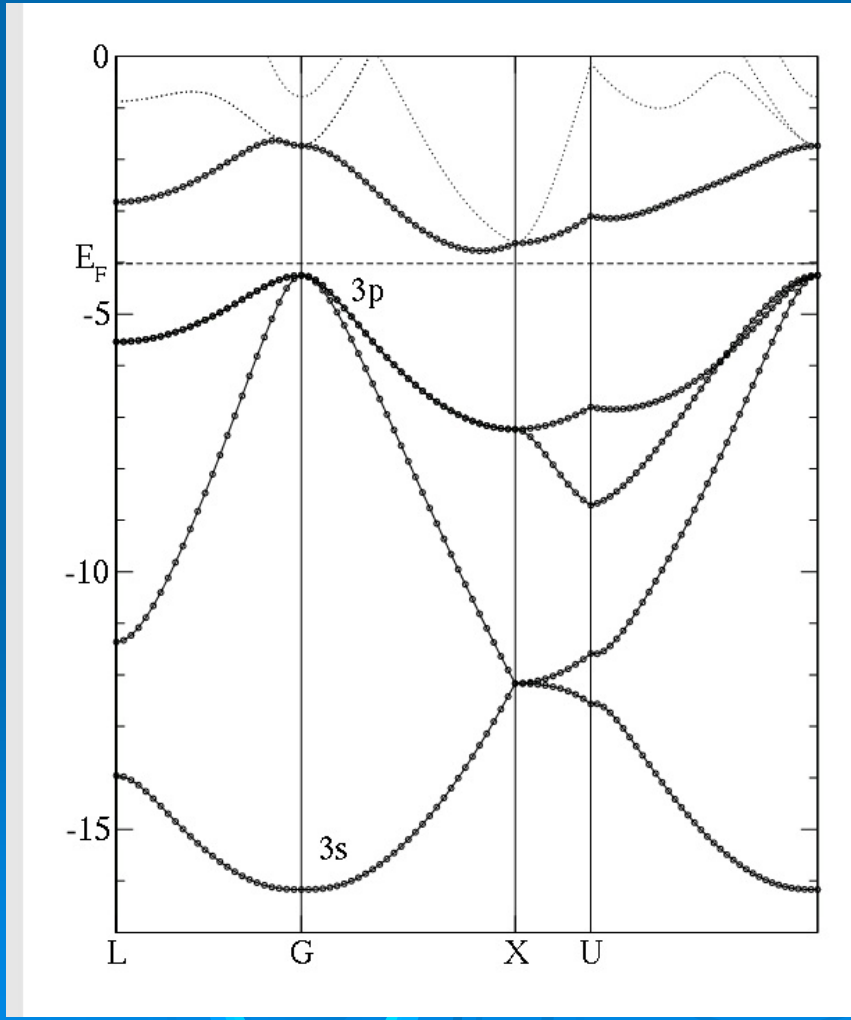
```
MeshCutoff            40.0 Ry        # Energy cut-off for 3D mesh

kgrid_cutoff  25.0 Bohr              # Grid of k-points

MaxSCFIterations     50              # Max. number of iterations in SCF.
DM.MixingWeight       0.3            # weight of mixing in the DM for convergence
DM.NumberPulay        3              # Number of previous steps of DM for mixing
DM.Tolerance          1.d-3          # Tolerance in differences of DM
DM.UseSaveDM
ElectronicTemperature  25 meV

SolutionMethod        diagon         # diagonalizacion, order-N, TD-DFT

XC.functional         LDA            # flavour of functional (LDA/GGA)
XC.authors            CA             # Parametrization fos xc
SpinPolarized         .false.        # spin polarization

MD.TypeOfRun             cg          # Molecular Dynamic options
MD.VariableCell       .true.
MD.NumCGsteps            30

WriteEigenvalues     .true.
WriteKbands          .true.
WriteBands           .true.
WriteWaveFunctions   .true.
WriteMullikenPop     1

%block BandLines
     1  1.000  1.000  1.000  L        #
    25  0.000  0.000  0.000  \Gamma   #
    30  2.000  0.000  0.000  X        #
    10  2.000  0.500  0.500  U        #
    35  0.000  0.000  0.000  \Gamma   #
%endblock BandLines

%block WaveFuncKPoints               # Weights of orbitals for bands in k-point
 0.000  0.000  0.000  from 1 to 20    # k-point, and bands required.
%endblock WaveFuncKPoints
                                                          66,1          Bot
```

# Plot bandstructure



# Instructions (III)

- See in the output file, or using silicon.WFS, the contributions of each orbitals to the bands at Γ:
  - Open “input.wfs”

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```
silicon.WFS
silicon.wfs.dat
0.1
~
```

  - Execute readwf

```
readwf < input.wfs
```

  - The ouput is in silicon.wfs.dat

# Instructions (IV)

- Plot the Density Of States (DOS)
  - Modify the silicon.EIG file
  - Use the eig2dos utility

```
eig2dos < silicon.EIG | tee dos,dat
```

  - Plot the data
    - `xmgrace dos.dat &`
    - Select the range of energies

# silicon.EIG

Fermi level  # k-points

add: "eta", "ne", "emin", "emax"

# bands

# Spin components

```
File   Edit   View   Terminal   Go   Help
      -3.7315
   26      1      4
   1   -15.43290    -8.21479    -5.04898    -5.04898    -2.33432    -0.71705
-0.71705     2.88446     3.29288     3.29288
         6.88751     8.96059    11.48087    11.48087    16.52234    16.52234
19.63799    23.59331    23.59331    30.27714
        30.75135    30.75135    38.09419    53.21218    53.21218    63.75667
   2   -13.53381   -10.75424    -7.85719    -6.55860    -2.79448     0.26363
 1.56871     1.82835     6.11173     6.74553
         8.41376     8.63656    11.07137    14.22357    15.27920    15.55248
17.43106    19.63489    21.27924    25.07139
        25.34765    33.30966    37.19144    45.92704    48.30519    92.49008
   3   -13.53381   -10.75424    -7.85719    -6.55860    -2.79448     0.26363
 1.56871     1.82835     6.11173     6.74553
         8.41376     8.63656    11.07137    14.22357    15.27920    15.55248
17.43106    19.63489    21.27924    25.07139
        25.34765    33.30966    37.19144    45.92703    48.30519    92.49009
   4   -13.53381   -10.75424    -7.85719    -6.55860    -2.79448     0.26363
 1.56871     1.82835     6.11173     6.74553
         8.41376     8.63656    11.07137    14.22357    15.27920    15.55248
17.43106    19.63489    21.27924    25.07139
        25.34765    33.30966    37.19144    45.92703    48.30519    92.49009
```

K-point, $e_1$, $e_2$, …, $e_n$

# Instructions (IV)

- Plot the Density Of States (DOS)
  - Modify the silicon.EIG file
  - Use the eig2dos utility

```
eig2dos < silicon.EIG | tee dos,dat
```

  - Plot the data
    - `xmgrace dos.dat &`
    - Select the range of energies

# Instructions (V)

- Write down the energy.
- Repeat the siesta run with different grids:
  - Edit the fdf, changing MeshCutoff to 40, 50, 80, 100, 120, 180 and 260 Ry. Write down the total energies.
  - Check in the output file the real value of the MeshCutoff used in each calculation.
  - Plot the Energy vs. MeshCutoff, to see the convergence

# Instructions (VI)

- Write down the energy.
- Repeat the siesta run with different kgrid_cutoff:
  - Edit the fdf, changing kgrid_cutoff to 5, 10, 15, 20, 25, 30 , 35, 40 and 45 bohr. Write down the total energies.
  - Check in the output file the number of k-points used in each calculation.
  - Plot the Energy vs. # k-points, to see the convergence