Introduction to SIESTA

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*  WELCOME TO SIESTA  *
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James Sifuna
George Manyali
George Amolo

Major reference in this lecture

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The SIESTA method for *ab initio* order-N materials simulation

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Computational methods

In condensed matter physics, they are a powerful tool for predicting and explaining properties in:

- Materials
- Nanostructures
- Small biological systems

Density functional theory has become a standard for simulations at the atomic and nanometric scales

Several numerical implementations of DFT are available.

- GNL
- Commercial

DFT CODE

Basis function used

- Plane waves
  - VASP
  - Q. ESPRESSO
  - ABINIT
  - CASTEP
  - CP2K
- Numerical orbitals
  - SIESTA
  - OpenMX
  - CRYSTAL
  - QUEST
  - ABRED
  - FIREBALL
  - PLATO

The choice of the electrons to be used

- Core + valence
  - *All electron codes*
    - WIEN2K
    - ELK
    - EXCITING
- Valence
  - *Pseudopotential codes*
    - Most codes

The list is not exhaustive, there are many other codes not mentioned in this talk

SIESTA

We will provide an over view in:

Installation

Make an input

Run a calculation

Make analysis

We will demonstrate using silicon

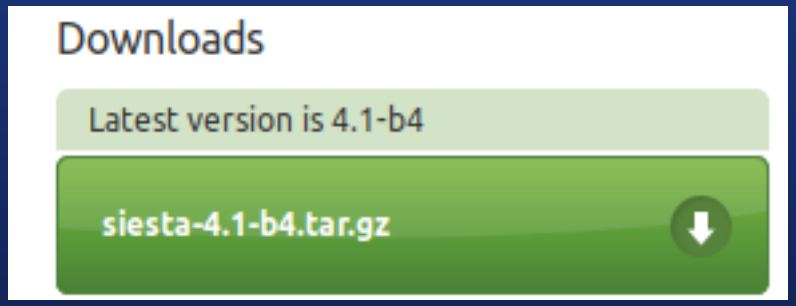
In this case we have converged the system for you to ease the process.

We will fit to an Equation of state
and
also obtain the bandstructure

Installation of a stable version

https://launchpad.net/siesta

Download version 4.1



gunzip then untar

cd **siesta-4.1-b4/Obj**

sh ../Src/obj_setup.sh

cp **gfortran.make arch.make**

make

After some few minutes you shoud have the siesta executable with you

Try this **./siesta**

You should see

```
***********************
*  WELCOME TO SIESTA  *
***********************
```

Requirements for a calculation

Before running SIESTA you require :

- **An access to the executable**
- **An input file (.fdf)**
- **A pseudopotential**

Pseudopotential types:

- **.psml**
- **.vps**
- **.psf**

FDF- flexible data format language: Characterized by,

- Data can be given in any order!
- Data can be omitted in favor of defaults
- Labels are case insensitive: characters like - _ . are ignored!
- Character strings not in apostrophes

Silicon input

As I said earlier, we have optimized the crystal structure to save your time and learn

We will describe a silicon input file here.

```
SystemName              bulk silicon
SystemLabel             si

NumberOfAtoms           2
NumberOfSpecies         1

%block ChemicalSpeciesLabel
 1  14  Si
%endblock ChemicalSpeciesLabel

PAO.BasisSize           DZP
PAO.EnergyShift         300 meV

LatticeConstant         5.43 Ang
%block LatticeVectors
  0.00  0.50  0.50
  0.50  0.00  0.50
  0.50  0.50  0.00
%endblock LatticeVectors
```

Descriptive name

Nickname for the outputs

No. of atoms in the simulation

No. of different atomic species

Specifies the different chemical species

pseudoatomic orbitals for each *l*

Length for scale

Will be read as a matrix

MUST be defined!

Silicon input continued

```
MeshCutoff                700.0 Ry

MaxSCFIterations          50
DM.MixingWeight           0.3
DM.NumberPulay            3
DM.Tolerance              1.d-4

kgridcutoff               7. Ang

SolutionMethod            diagon
ElectronicTemperature     25 meV

%block kgrid_Monkhorst_Pack
  11  0  0  0.5
  0  11  0  0.5
  0  0  11  0.5
%endblock kgrid_Monkhorst_Pack
```

Energy cutoff

Can be ignored in favor of default values

Fictitous temperature for smearing!

Mesh grid size

Silicon input continued

```
BandLinesScale  pi/a
%block BandLines
 1  0.000  0.000  0.000  \Gamma
25  2.000  0.000  0.000     X
10  2.000  1.000  0.000     W
15  1.000  1.000  1.000     L
20  0.000  0.000  0.000  \Gamma
25  1.500  1.500  1.500     K
%endblock BandLines
AtomicCoordinatesFormat  Fractional
%block AtomicCoordinatesAndAtomicSpecies
    0.     0.     0.      1       Si         1
    0.25   0.25   0.25    1  Si       2
%endblock
AtomicCoordinatesAndAtomicSpecies
%block ProjectedDensityOfStates
  -70.00  5.00  0.150 3000  eV
%endblock ProjectedDensityOfStates

%PDOS.kgrid_Monkhorst_Pack
   60  0  0  0.5
    0 60  0  0.5
    0  0 60  0.5
%end PDOS.kgrid_Monkhorst_Pack
```

High symmetry points in the Brillouin zone

FDF language permits any order of data. This are the atomic positions

Dense grid grid to perform the PDOS calculation

See input attached!!!!!!!

Run the calculation

We will perform an scf calculation which will later on be followed by the band structure calculation.

Proceed as follows:

- **Copy the si.fdf and the si.psf (input and the pseudopotential) in a preferred folder.**
- **~/siesta <si.fdf | tee si.out**
- **After a successful run, you will find too much data printed.**
- **I will be interested in si.PDOS and si.bands**

At this point, we will do post processing of the output.

gnubands.f

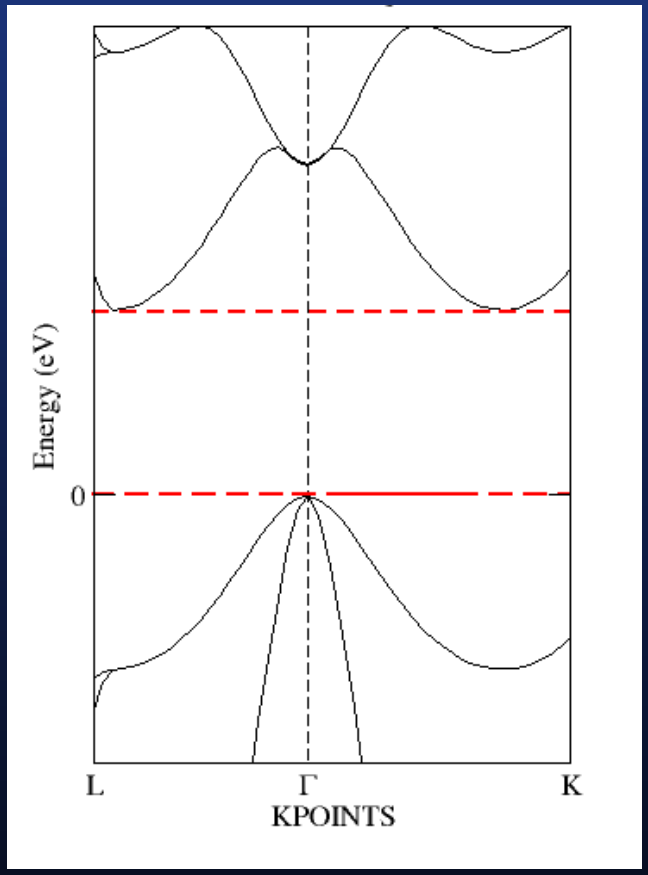
fmpdos

Scripts that I have attached and are key in bands and PDOS extraction

Band structure for silicon

Proceed as follows for the bands

- **gfortran -o gnubands.x gnubands.f**
- **./gnubands.x <si.bands> siliconbands.dat**
- **Plot the gnubands.x using your prefered plotter**



For the pdos:

Proceed as follows:

./fmpdos then follow the instructions!