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MAX DRIVING THE EXASCALE TRANSITION

siesta On-line School 2024

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# Analysis tools

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# Charge analysis

## Background

N electronic states

$$n(r) = \sum_{i}^{N} |\psi_i^{KS}(r)|^2$$

## Basis Expansion:

M basis functions

$$|\psi_i\rangle = \sum_{\mu=1}^{M} c_{i,\mu} \, |\mu\rangle$$

$$\int_{\Omega} n(r) = N = \sum_{i}^{N} \langle \psi_i | \psi_i \rangle = \sum_{i} \sum_{\mu\nu} c_{i\mu}^{*} c_{i\nu} \langle \mu | \nu \rangle = \sum_{\mu\nu} \rho_{\mu\nu} S_{\mu\nu}$$

Density matrix

$$\rho_{\mu\nu} = \sum_{i} c_{i\mu}^{*} c_{i\nu}$$

Overlap matrix

$$S_{\mu\nu} = \langle \mu | \nu \rangle$$

# Charge analysis

N electronic states

$$n(r) = \sum_{i}^{N} |\psi_i^{KS}(r)|^2$$

## Basis Expansion:

M basis functions

$$|\psi_i\rangle = \sum_{\mu=1}^{M} c_{i,\mu} \, |\mu\rangle$$

$$\int_{\Omega} n(r) = N = \sum_{i}^{N} \langle \psi_i | \psi_i \rangle = \sum_{i} \sum_{\mu\nu} c_{i\mu}^{*} c_{i\nu} \langle \mu | \nu \rangle = \sum_{\mu\nu} \rho_{\mu\nu} S_{\mu\nu}$$

$$N = \sum_{I} q_I = \sum_{I} \sum_{\mu \in I} \sum_{\nu} \rho_{\mu\nu} S_{\mu\nu}$$

## Mulliken charges

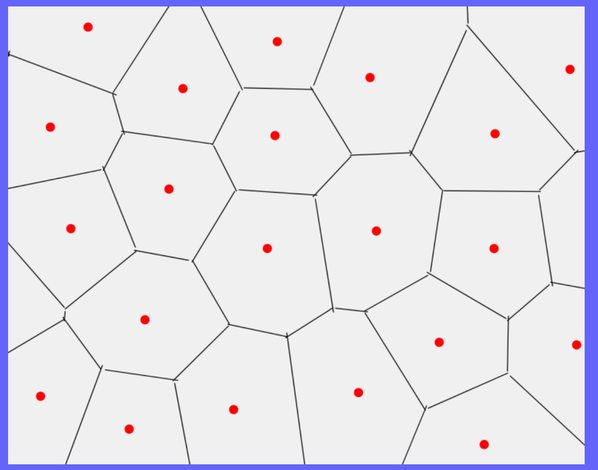
`WriteMullikenPop` 0/ 1 / 2 / 3

# Charge analysis

$$\int_{\Omega} n(r) = N = \sum_{I} \int_{\Omega_I} n(r)$$

## Voronoi charges

```
Write.VoronoiPop        True
```

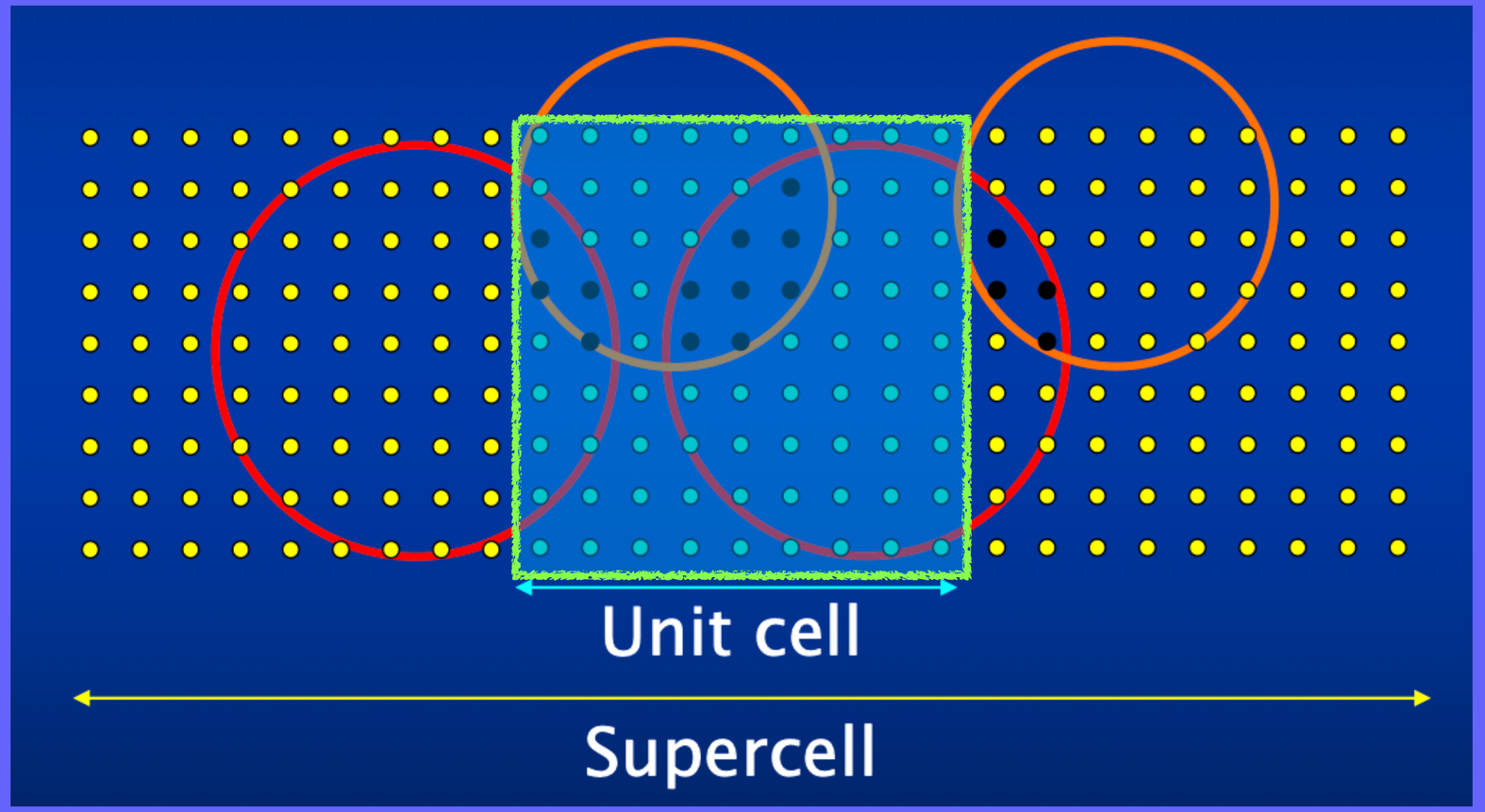


$$q_I = \int_{\Omega} dr \frac{\rho^I_{atom}(r)}{\sum_J \rho^J_{atom}(r)} n(r)$$

## Hirshfeld charges

```
Write.HirsfeldPop       True
```

# Charge densities and potentials on grid

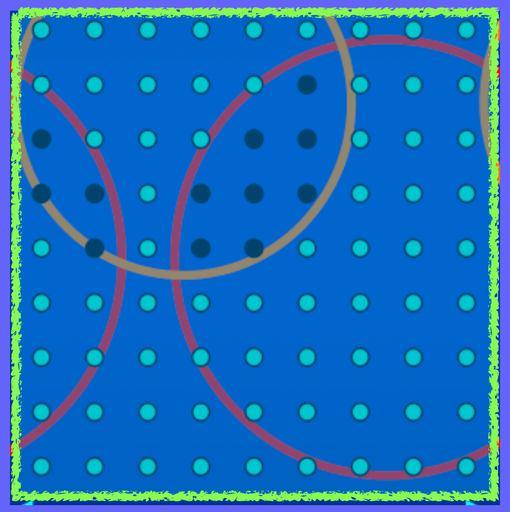



$N_1 \times N_2 \times N_3$ mesh points... $F(i,j,k) \longrightarrow F(n)$

# Charge densities and potentials on grid

Possible F(n)?

- RHO $\rho(r) = \sum_{\mu,\nu} \rho_{\mu\nu} \phi_\mu(r) \phi_\nu(r)$
- DRHO $\delta\rho(r) = \rho_{SCF}(r) - \rho_{atom}(r)$
- VT $V_{SCF}(r)$
- VH $\delta V_H(r)$



- SaveRho
- SaveDeltaRho
- SaveTotalPotential
- SaveElectrostaticPotential

$N_1 \times N_2 \times N_3$ mesh points... F(i,j,k) $\longrightarrow$ F(n)

# Charge densities and potentials on grid

Possible F(n)?

- LDOS $n(\epsilon, r) = \sum_n |\psi_n(r)|^2 \delta(\epsilon - \epsilon_n)$

$$LDOS(r) = \int_{\epsilon_1}^{\epsilon_2} n(\epsilon, r)$$

```
%block LocalDensityOfStates
   EF  -3.50   0.00  eV
%endblock LocalDensityOfStates
```

- Wavefunctions $|\psi_n(r)|^2$ $\psi_n(r)$ Real, Imag, Mod, Phase

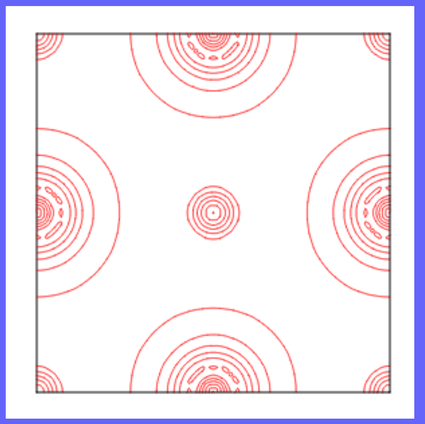
$N_1 \times N_2 \times N_3$ mesh points... F(i,j,k) $\longrightarrow$ F(n)

# Charge densities and potentials on grid

Utils that might be useful

- Util/Grid/
  - grid2cdf, cdf2grid
  - cdf2xsf
  - cdf_diff
  - cdf_laplacian
  - grid2val
  - grid2cube
  - grid_rotate

- Util/Contour
  - grid1d (?)
  - grid2d



- Util/Plrho

- Util/Denchar/

https://docs.siesta-project.org/projects/siesta/en/5.2/reference/denchar.html

- SISL

# Charge densities and potentials on grid

## Utils that might be useful

- `Util/Contrib/FElMellouhi`
  - Conversion to openDX format
- `Util/Contrib/APostnikov`
  - rho2xsf
  - (+ eig2bxsf + vib2xsf + etc)

# Visualisation GUI tools

XCrySDen

X-window CRYstalline Structures and DENsities

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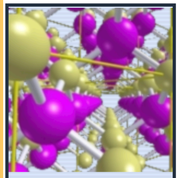

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## XCrySDen

*XCrySDen* is a **crystalline and molecular structure visualisation program** aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. It runs on GNU/Linux.

*XCrySDen* has been also ported to Mac OS (requires X11) and Windows (requires either CYGWIN or WSL).

The name of the program stands for *Crystalline Structures and Densities* and *X* because it runs under the X-Window environment.

Read more... | See screenshots ...

**Latest version:** 1.6.2

### XCrySDen mailing list

*XCrySDen* mailing list is an open mailing list where XCrySDen related issues can be discussed among users.

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VESTA

Visualization for Electronic and STructural Analysis

Software > VESTA

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Topaz

### 1. Introduction

VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below.

- Deal with multiple structural models, volumetric data, and crystal morphologies in the same window.
- Support multiple tabs corresponding to files.
- Support multiple windows with more than two tabs in the same process.
- Deal with virtually unlimited number of objects such as atoms, bonds polyhedra, and polygons on isosurfaces (theoretical limit on 32bit operating system is 1,073,741,823)
- Support lattice transformation from conventional to non-conventional lattice by using matrix. The transformation matrix is also used to create superlattice and sublattice.
- Visualize interatomic distances and bond angles that are restrained in Rietveld analysis with RIETAN-FP.
- Transparent isosurfaces can be overlap with structural models.

## The GDIS Home Page

GDIS
Modeling Interface

Snapshot 1
Snapshot 2
Snapshot 3
Snapshot 4
Download

Author:
*Sean Fleming*

*Introduction*

GDIS is a GTK based program for the display and manipulation of isolated molecules and periodic systems. It is in development, but is nonetheless fairly functional. It has the following features:

- Support for several file types (CIF, BIOSYM, XYZ, XTL, MARVIN, and GULP)
- OpenGL rendering (requires gtkglarea)
- Assorted tools for visualization (measurements, ribbons, polyhedral display)
- Useful manipulation tools, including matrix transformations and periodic image display.
- Powerful surface generation and crystal morphology tools.
- Animation of BIOSYM and GULP trajectory files

GDIS also allows you to perform the following functions through other packages:

- Model rendering (courtesy of POVRay)
- Energy minimization (courtesy of GULP)
- Morphology calculation (courtesy of cdd)
- Space group processing (courtesy of SeInfo)
- View the Periodic Table (courtesy of GPeriodic)
- Load additional filetypes, such as PDB (courtesy of Babel)

Although developed on a RedHat Linux platform, GDIS has been successfully compiled under IRIX, Solaris, OpenBSD, and OS-X. I've even built a Window's executable using the mingw32 cross-compiler!

The source code is released under the GPL.

Molekel

Molecular visualization

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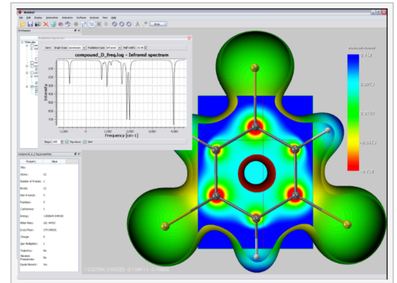
## Molekel

Molekel is an open-source multi-platform molecular visualization program.

(citation info)

Some of the features available in the new version are:

- Multiplatform: Mac OS X, Windows, Linux
- Different methods to speed-up rendering of molecules with support for billboards and view-dependent level of detail techniques
- Programmable shaders; standard shaders to enhance rendering quality, outline contours and perform sketch-like renderings are provided
- Visualization of residues (ribbon or schematic)

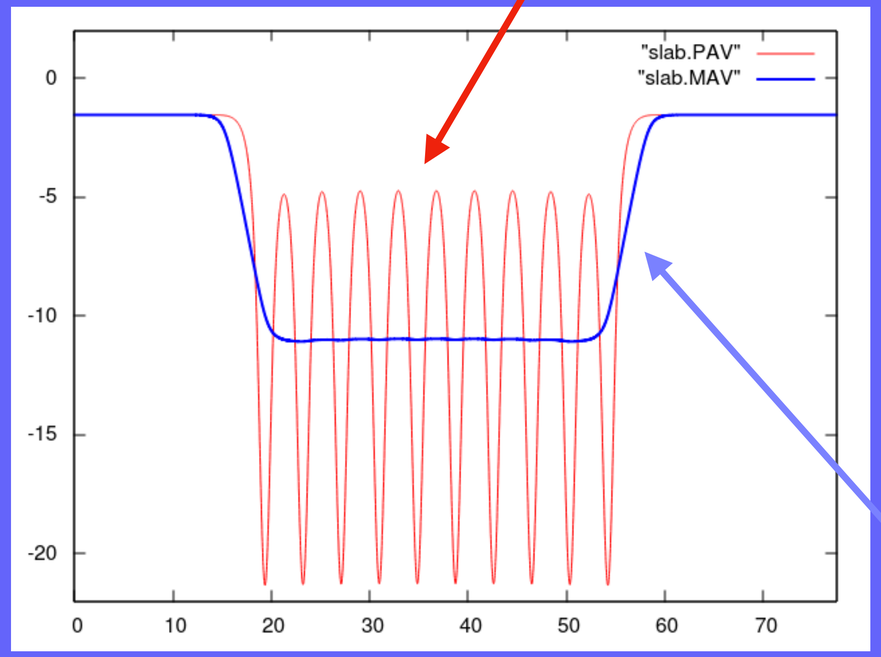


Click on image to enlarge

# Macroscopic averages of grid functions

## MACROAVE (`siesta/Util/Macroave`)

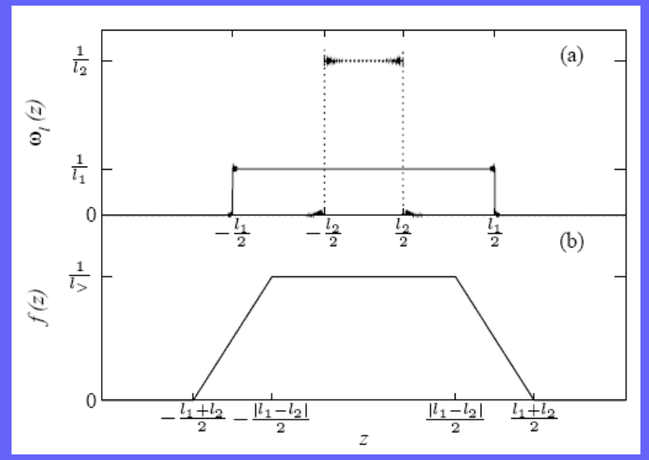
$$\overline{F}(z) = \frac{1}{S}\int_S dxdy\, F(x,y,z)$$




Atomic scale fluctuations can be washed out by convolution with a filter function

$$\Theta(z-z') = \int dz''\omega_{l_1}(z-z'')\,\omega_{l_2}(z''-z')$$

$$\overline{\overline{F}}(z) = \int dz'\Theta(z-z')\overline{F}(z')$$



# How to use macroave?

1) Run SIESTA to extract the grid-function you want to analyse.

| FDF flags | | Output files |
|---|---|---|
| SaveRho | .true. | SystemLabel.RHO |
| SaveDeltaRho | .true. | SystemLabel.DRHO |
| SaveElectrostaticPotential | .true. | SystemLabel.VH |
| SaveTotalPotential | .true. | SystemLabel.VT |
| SaveTotalCharge | .true. | SystemLabel.TOCH |
| SaveIonicCharge | .true. | SystemLabel.IOCH |
| … | | |

2) Edit the input file macroave.in (see next)

3) Execute the code: `$path/to/your/executable/macroave.x`

# How to use macroave?

Input file: `macroave.in`

```
siesta                  # Which code have you used to get the input data?
charge                  # Which is the input data used to compute the band offset?
slab                    # Name of the file where the input data is stored
1                       # Number of convolutions required to calculate the macro. ave.
4.200                   # First length for the filter function in macroscopic average
4.000                   # Second length for the filter function in macroscopic average
330                     # Total charge
spline                  # Type of interpolation
```

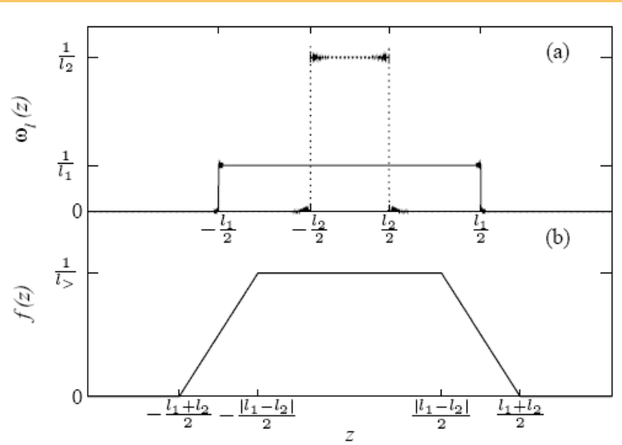
1) siesta / abinit

2) Potential / Charge / TotalCharge

3) 1 for surfaces / 2 for interfaces

4) total number of electrons (used to renormalise charge)

5) Spline / linear



# How to use macroave?

## Output files:

`SystemLabel.PAV`

Planar average

$$\overline{F}(z) = \frac{1}{S}\int_S dxdy\, F(x,y,z)$$

`SystemLabel.MAV`

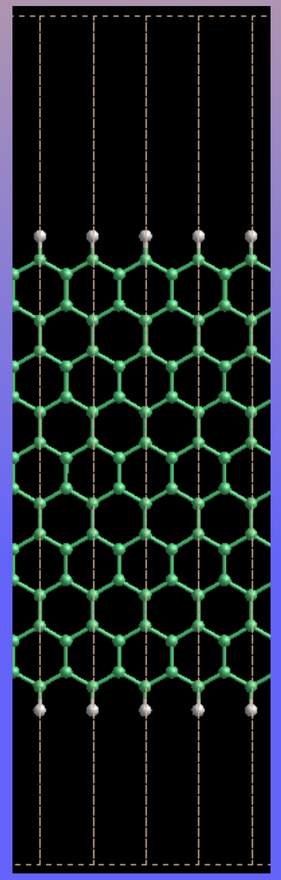
Nanosmoothed

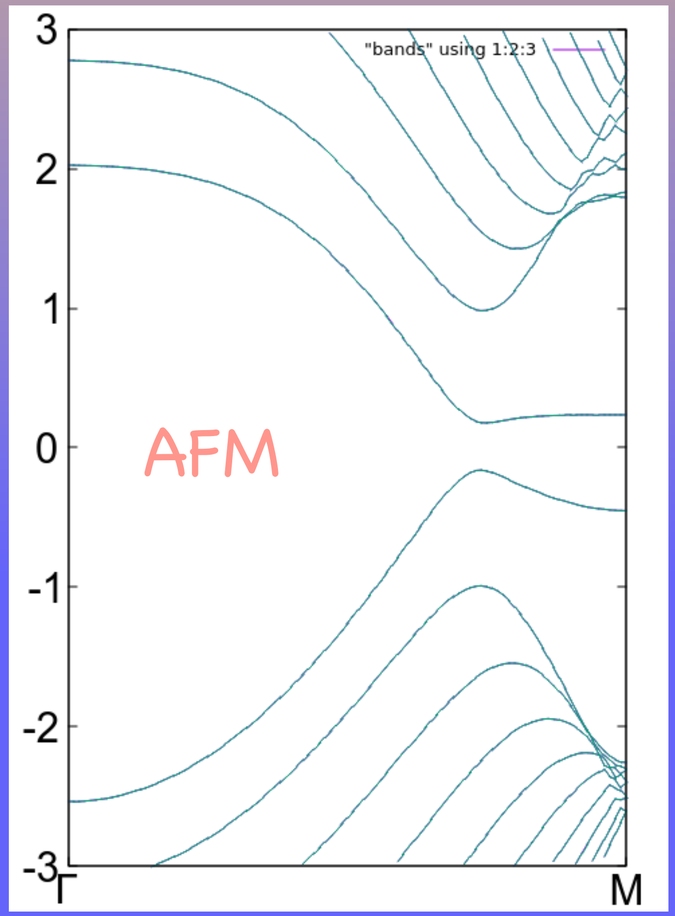
$$\overline{\overline{F}}(z) = \int dz' \Theta(z-z')\overline{F}(z')$$

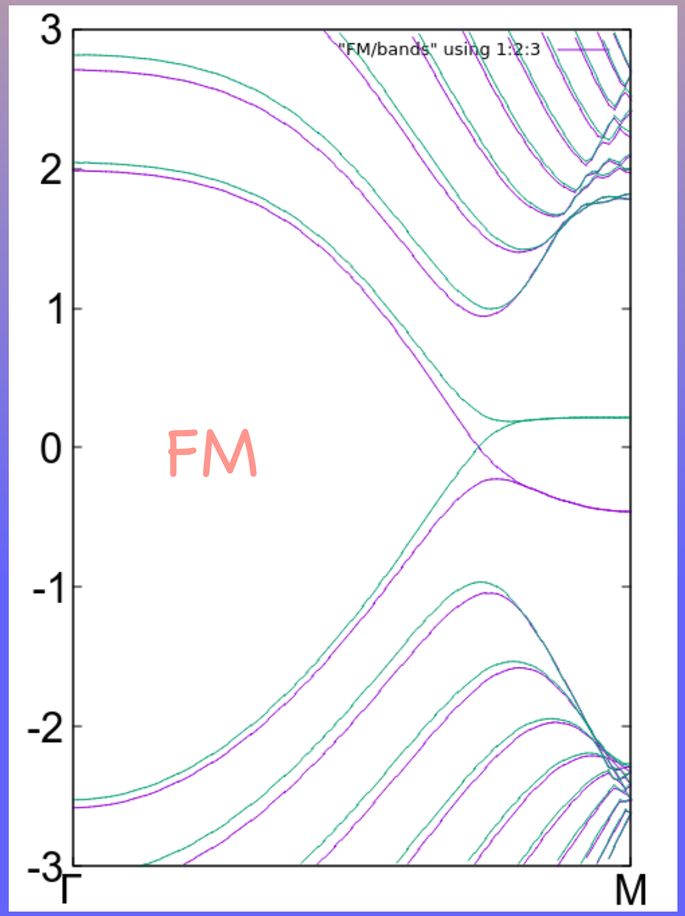
**Units:**

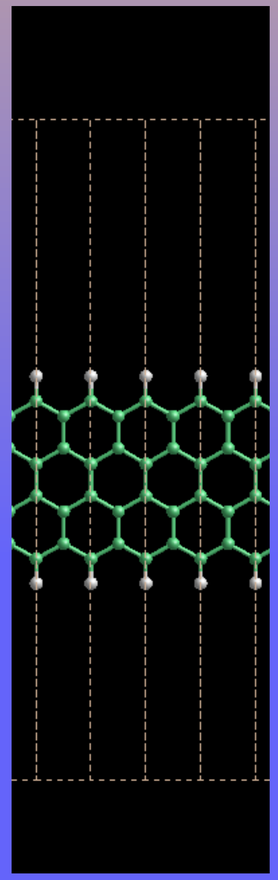
- Coordinates in Bohr
- Potential in eV
- Charge density in electrons/Bohr$^3$

# Hands-on tutorial: plotting DOS & bands in zGNR





10-zgnr

4-zgnr

```
%block DM.InitSpin
   Cedge1    +
   Cedge2    -
%endblock DM.InitSpin
```

# Hands-on tutorial: plotting DOS & bands in zGNR

```
WriteKbands         .true.
WriteBands          .true.
BandLinesScale     ReciprocalLatticeVectors

%block Bandlines
  1    0.0000    0.0000    0.0000    \Gamma
100    0.5000    0.0000    0.0000    X
%endblock Bandlines
```

Generates a "SystemLabel.bands" file

Finally, use gnubands:

```
$ gnubands –help
```

## Density of States (DOS)

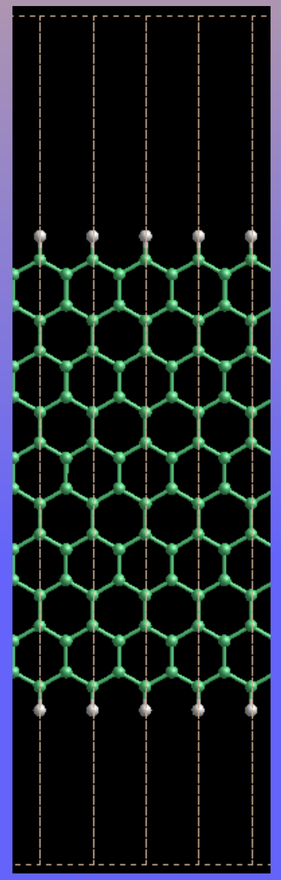
$$g(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i)$$

$$\delta \rightarrow e^{-(\varepsilon-\varepsilon_i)^2/\sigma^2}$$

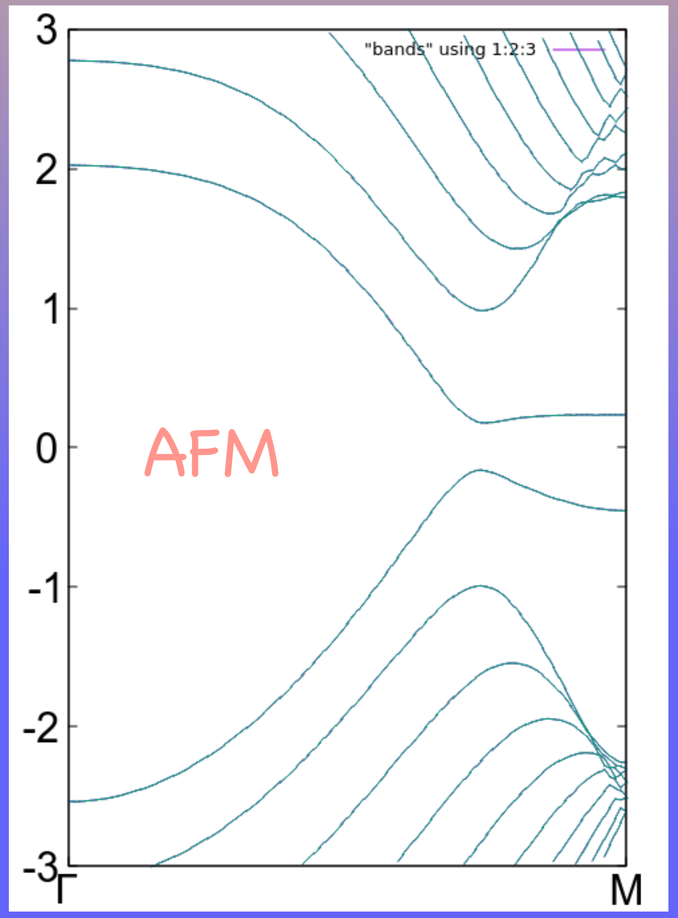
Take the "SystemLabel.EIG" file, and post process with Eig2DOS

```
$ Eig2DOS –help
```

# Hands-on tutorial: plotting DOS & bands in zGNR



10-zgnr




$$N = \sum_i f_i < \Psi_i | \Psi_i > = \sum_i f_i \sum_{\mu\nu} c_\mu^i c_\nu^i S_{\mu\nu}$$

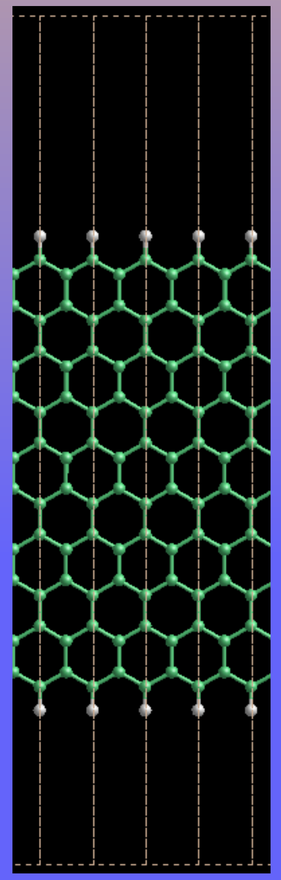
## Density of States (DOS)

$$g(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i) = \sum_i \sum_\mu \sum_\nu c_{i\mu} c_{i\nu} S_{\mu\nu} \delta(\varepsilon - \varepsilon_i)$$

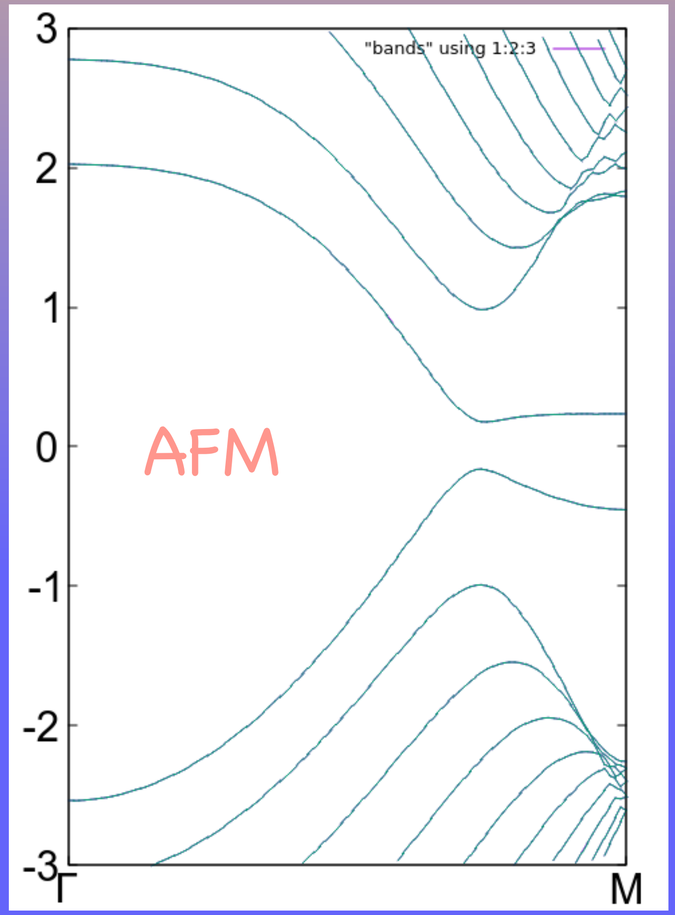
## Projected DOS on orbital $\mu$

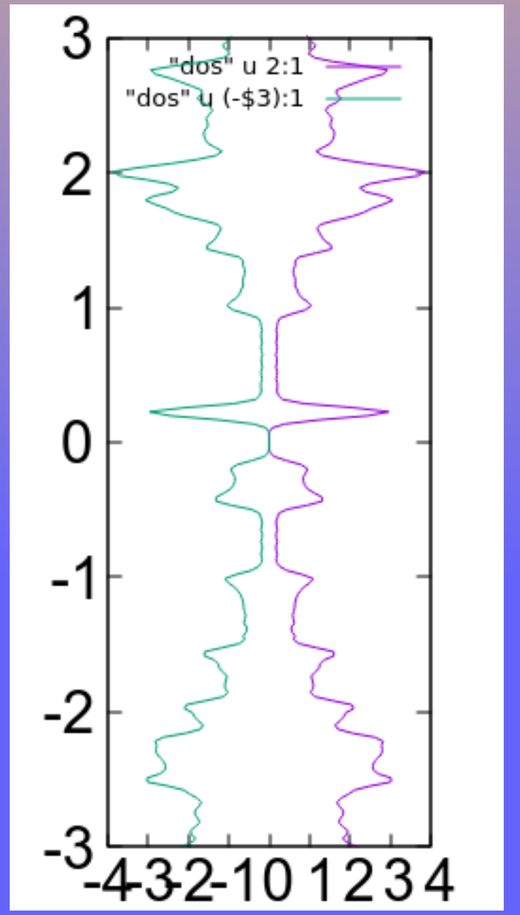
$$g_\mu(\varepsilon) = \sum_i \sum_\nu c_{i\mu} c_{i\nu} S_{\mu\nu} \delta(\varepsilon - \varepsilon_i)$$

# Hands-on tutorial: plotting DOS & bands in zGNR

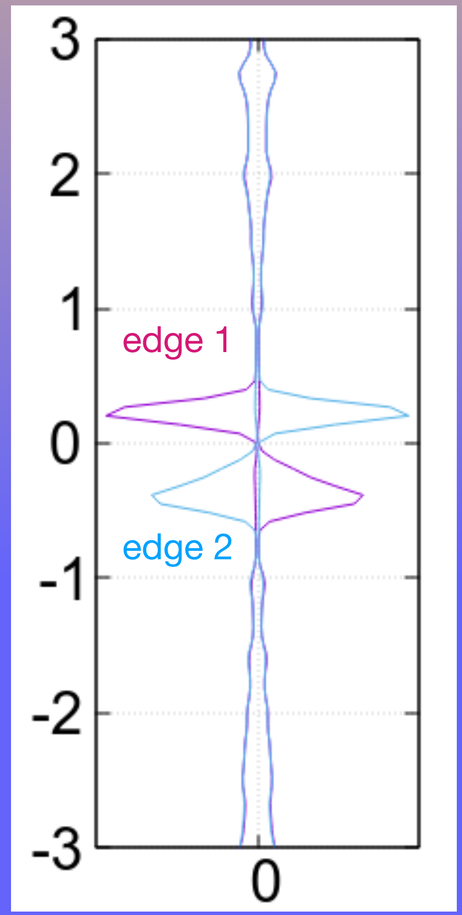


10-zgnr



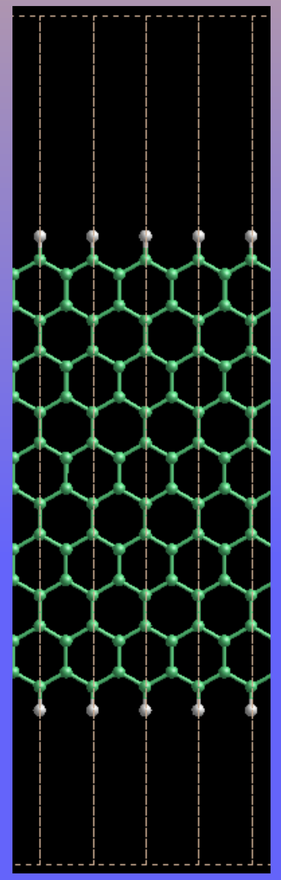




DOS

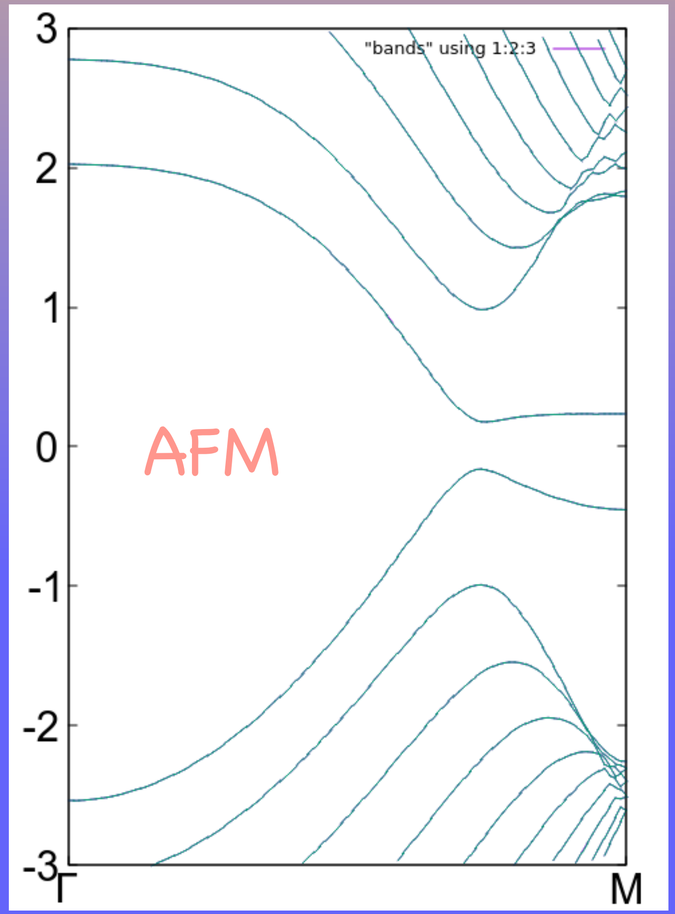


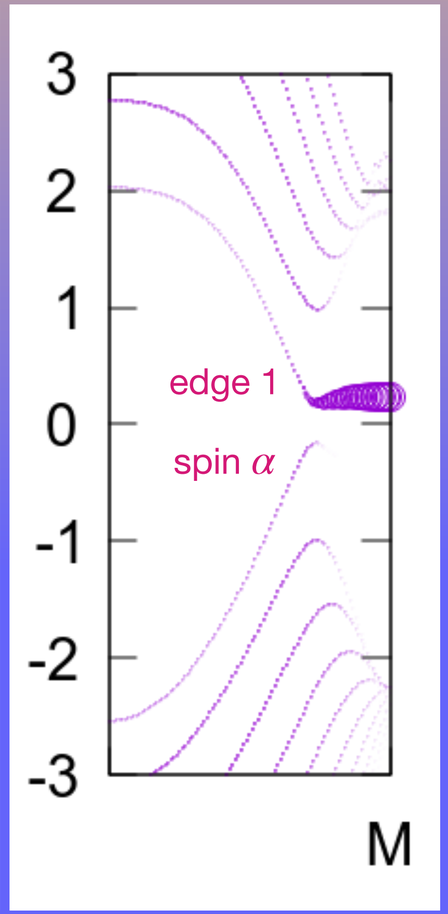

PDOS

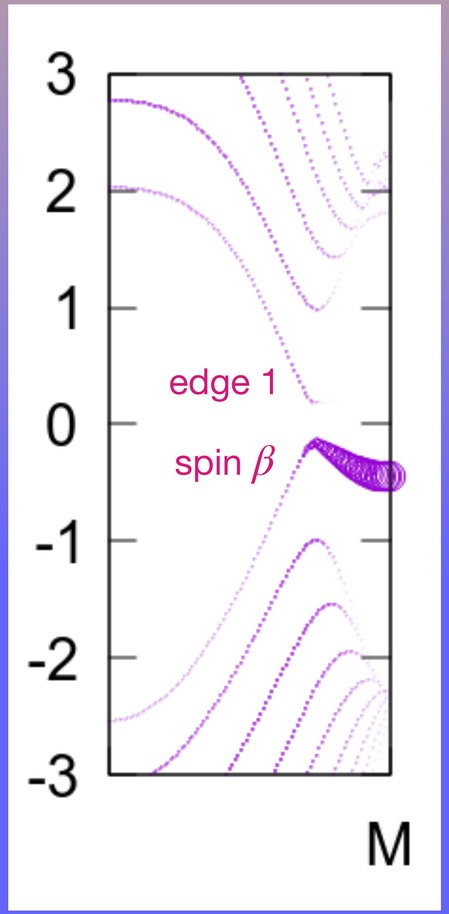
# Hands-on tutorial: plotting DOS & bands in zGNR



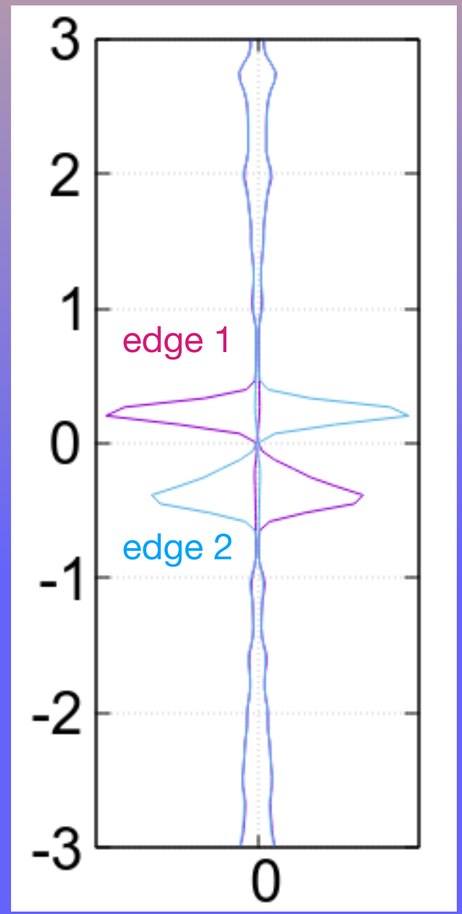
10-zgnr




Fatbands!!

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# Analysis tools

1) Copy your files from day2/05.AnalysisTools

2) Follow the instructions:

https://docs.siesta-project.org/projects/siesta/en/5.2/tutorials/basic/analysis-tools/index.html

3) Ask questions

CSIC

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