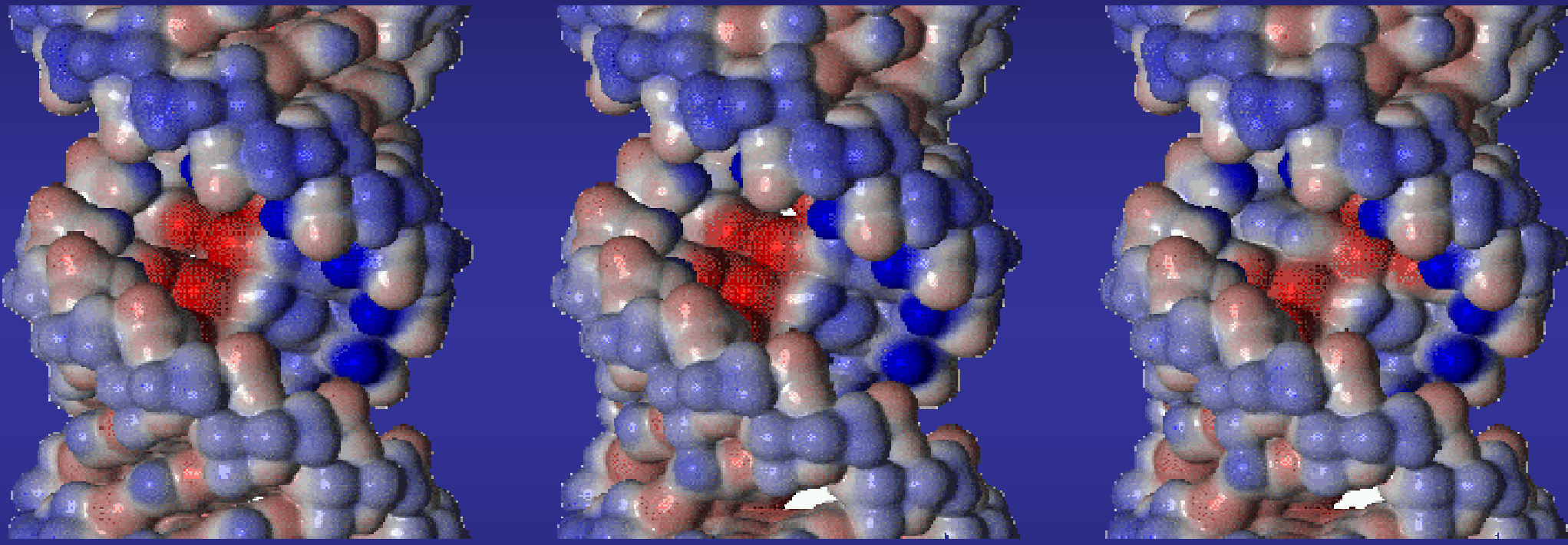
Analysis, post-processing and visualization tools



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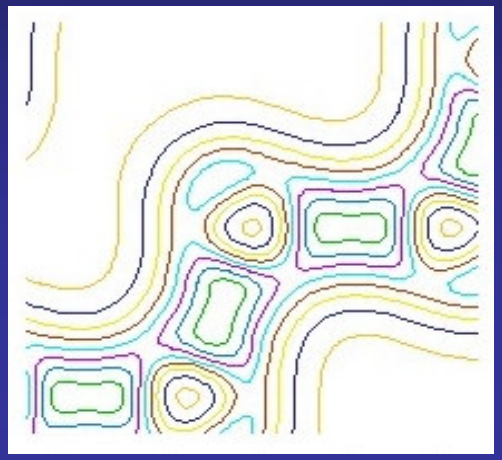
Andrei Postnikov

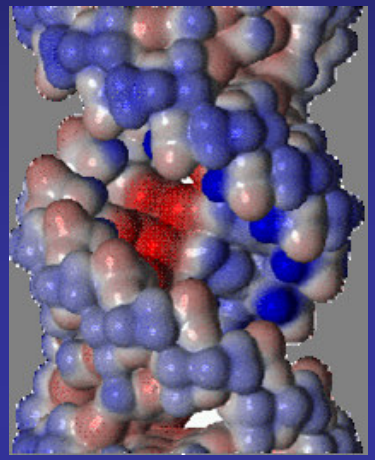
paul verlaine université - metz

Summary of different tools for post-processing and visualization

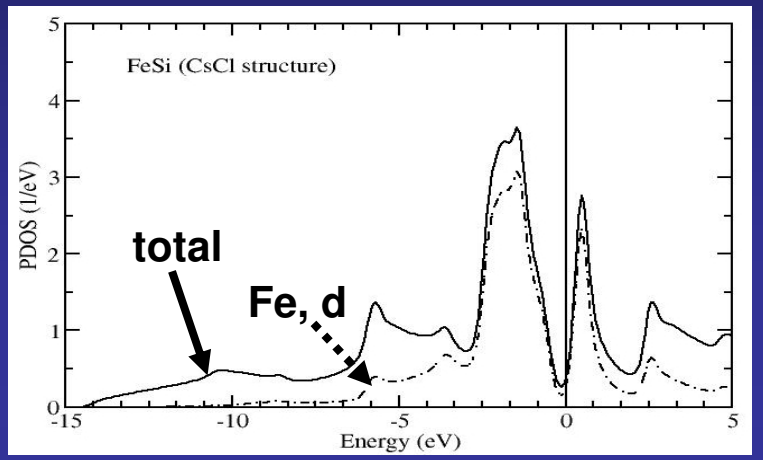
DENCHAR



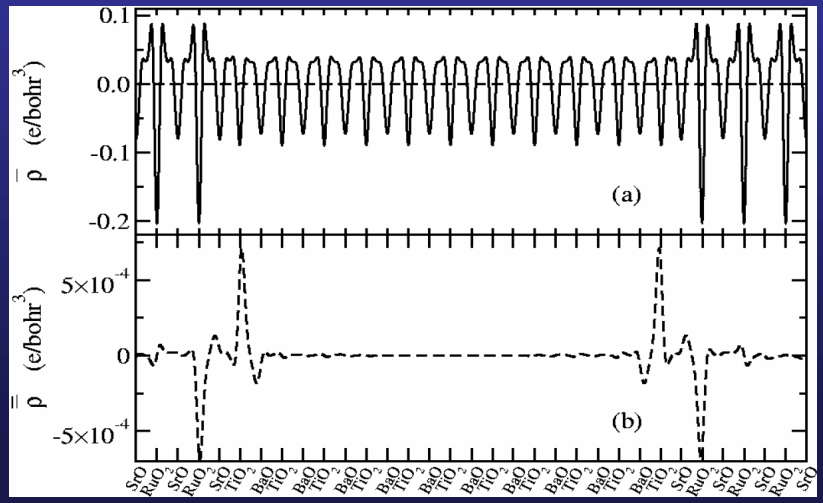
PLRHO



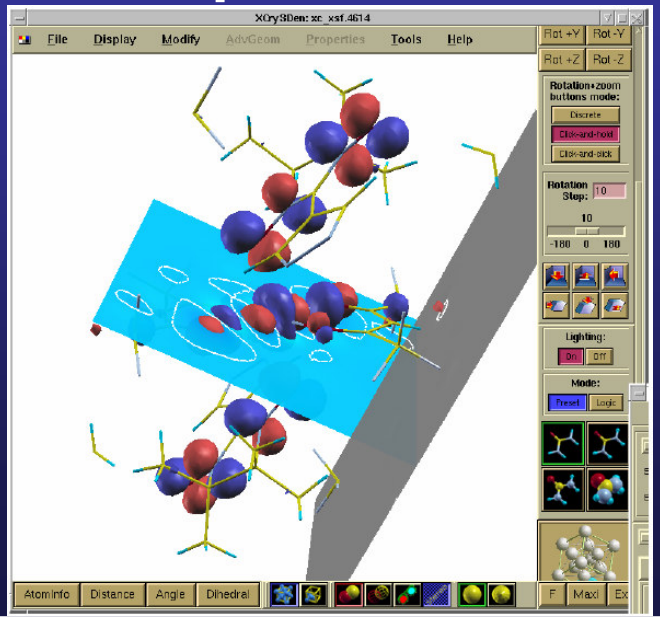
DOS, PDOS



MACROAVE

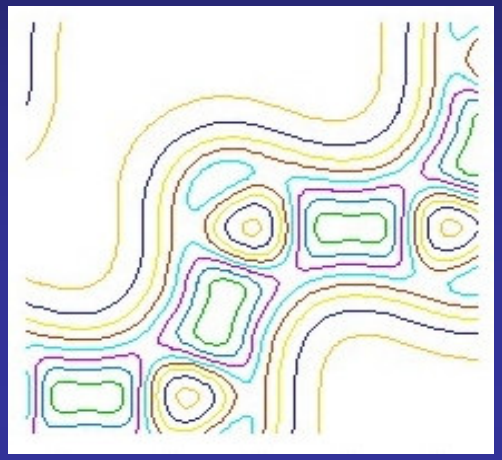


SIESTA's output with XCRYSDEN

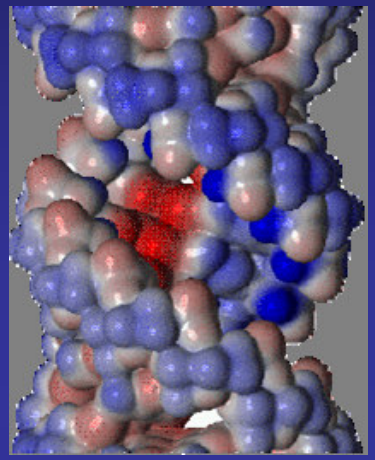


Summary of different tools for post-processing and visualization

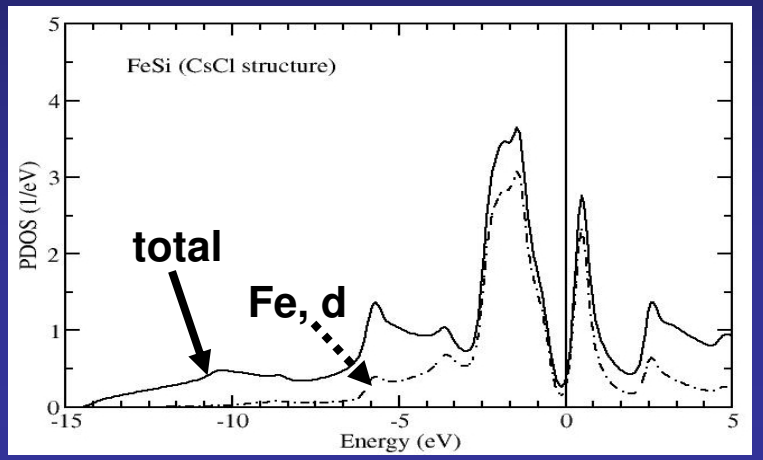
DENCHAR



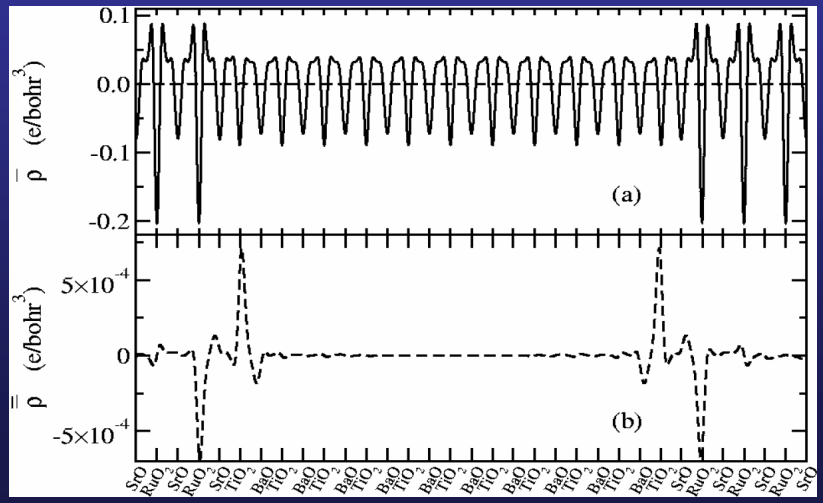
PLRHO



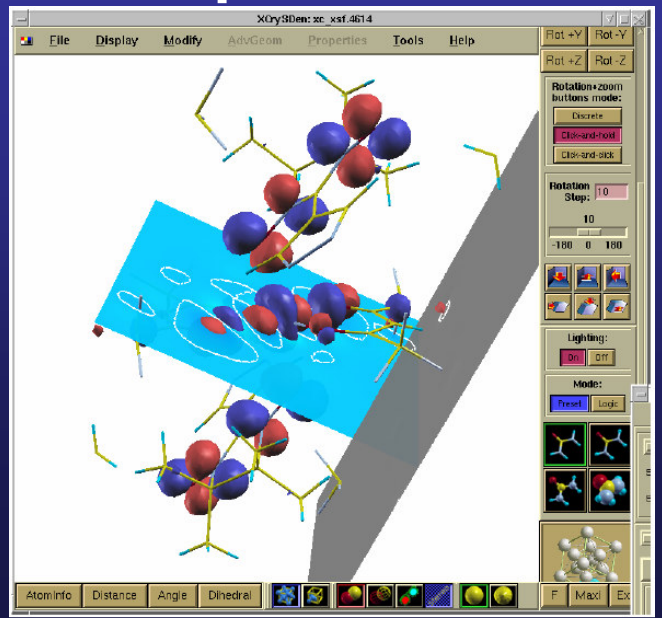
DOS, PDOS



MACROAVE



SIESTA's output with XCRYSDEN



DENCHAR plots the charge density and wave functions in real space

Wave functions

$$\psi_i(\vec{k},\vec{r}) = \sum_{\mu} e^{i\vec{k}\cdot\vec{R}_\mu} c_{\mu i}(\vec{k}) \phi_\mu(\vec{r})$$

Coefficients of the eigenvector $\psi_i(\vec{k})$ with eigenvalue $E_i(\vec{k})$

atomic orbitals

Charge density

$$\rho(\vec{r}) = \sum_i \int_{BZ} n_i(\vec{k}) \,|\, \psi_i(\vec{k},\vec{r}) \,|^2 d\vec{k}$$

$$= \sum_{\mu\nu} \rho_{\mu\nu} \phi^*_\nu(\vec{r}) \phi_\mu(\vec{r})$$

density matrix

DENCHAR operates in two different modes: 2D and 3D

2D

- Charge density and/or electronic wave functions are printed on a regular grid of points contained in a 2D plane specified by the user.
- Used to plot contour maps by means of 2D graphics packages.

3D

- Charge density and/or electronic wave functions are printed on a regular grid of points in 3D.
- Results printed in Gaussian Cube format.
- Can be visualized by means of standard programs (Moldel, Molekel, Xcrysden)

How to compile DENCHAR…

```
$ cd siesta/Src
$ make denchar
ifort -c -O3   f2kcli.F90
ifort -c -O3   m_denchar_init.F
ifort -c -O3   m_denchar_geom.f
ifort -c -O3   m_denchar_io.F
ifort -c -O3   m_denchar_neighb.f
ifort -c -O3   m_denchar_work.f
ifort -c -O3   denchar.F
ifort -o denchar \
            m_denchar_init.o m_denchar_geom.o m_denchar_io.o m_denchar_neighb.o
m_denchar_work.o denchar.o  precision.o recipes.o f2kcli.o bessph.o chkdim.o
dismin.o  dot.o iodm.o memory.o paste.o  radfft.o io.o  spatial.o volcel.o
parallel.o parallelsubs.o memoryinfo.o sys.o listsc.o atmparams.o atmfuncs.o
atm_types.o m_memory.o radial.o spher_harm.o  basis_io.o basis_types.o
pseudopotential.o chemical.o xml.o files.o bsd.o pxf.o \
            libfdf.a   linalg.a
```

Use the same arch.make file as for the compilation of serial SIESTA

Versions before 2.0.1, please check for patches in
http://fisica.ehu.es/ag/siesta-extra/issues.html

…and where to find the User's Guide and some Examples

```
$ cd siesta/Util/Denchar
$ ls
Docs  Examples  README-Source
```

How to run DENCHAR…

SIESTA

```
WriteDenchar                    .true.
WriteWaveFunctions              .true.
%block WaveFuncKPoints
     0.0  0.0  0.0
%endblock WaveFuncKPoints
```

} Only if you want to plot wave functions

Output of SIESTA required by DENCHAR

SystemLabel.PLD
SystemLabel.DIM
SystemLabel.DM
SystemLabel.WFS (only if wave functions)
ChemicalSpecies.ion (one for each chemical species)

DENCHAR

```
$ ln –s ~/siesta/Src/denchar .
$ denchar < dencharinput.fdf
```

You **do not** need to rerun SIESTA to run DENCHAR as many times as you want

Input of DENCHAR
General issues

- Written in fdf (Flexible Data Format), as in SIESTA
- It shares some input variables with SIESTA

  SystemLabel

  NumberOfSpecies

  ChemicalSpeciesLabel

- Some other input variables are specific of DENCHAR (all of them start with “Denchar.”)

  To specify the mode of usage

  To define the plane or 3D grid where the charge/wave functions are plotted

  To specify the units of the input/output

- Input of DENCHAR can be attached at the end of the input file of SIESTA

Input of DENCHAR
How to specify the mode of run

- **Denchar.TypeOfRun** (string) 2D or 3D

- **Denchar.PlotCharge** (logical) .TRUE. or .FALSE.

  If .true. SystemLabel.DM must be present

- **Denchar.PlotWaveFunctions** (logical) .TRUE. or .FALSE.

  If .true. SystemLabel.WFS must be present

Either one or the other (or both of them) must be .true.

Input of DENCHAR
How to specify the plane

Plane of the plot in 2D mode

x-y plane in 3D mode

- **Denchar.PlaneGeneration** (string)

  NormalVector

  TwoLines

  ThreePoints

  ThreeAtomicIndices

+ more variables to define the

  generation object (the normal vector, lines, points or atoms)

  origin of the plane

  x-axis

  size of the plane

  number of points in the grid

- Different variables described in the User Guide (take a look to the Examples)

Output of DENCHAR 2D mode

Charge density

Spin unpolarized:

- self-consistent charge (.CON.SCF)
- deformation charge (.CON.DEL)

Spin polarized:

- density spin up (.CON.UP)
- density spin down (.CON.DOWN)
- deformation charge (.CON.DEL)
- magnetization (.CON.MAG)

Wave functions

Wave function for different bands

(each wavefunction in a different file)

.CON.WF#, where # is the number of the wf

(If spin polarized, suffix .UP or .DOWN)

Format

x_i	y_i	$f(x_i, y_i)$
-5.00000	-5.00000	-0.00560
-5.00000	-4.74359	-0.00402
.	.	.
.	.	.

Output of DENCHAR 3D mode

Charge density

Spin unpolarized:

- self-consistent charge (.RHO.cube)
- deformation charge (.DRHO.cube)

Spin polarized:

- density spin up (.RHO.UP.cube)
- density spin down (.RHO.DOWN.cube)
- deformation charge (.DRHO.cube)

Wave functions

Wave function for different bands

(each wavefunction in a different file)

.WF#.cube, where # is the number of the wf

(If spin polarized, suffix .UP or .DOWN)

Format

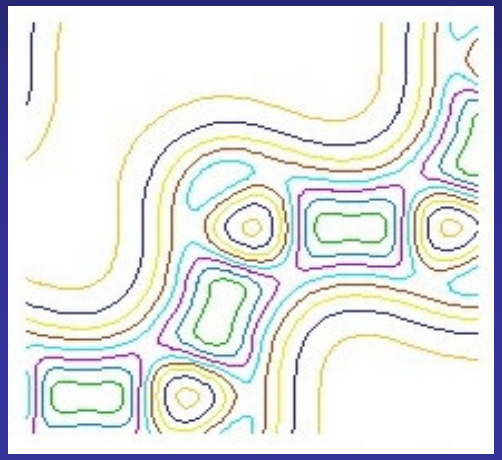
Gaussian Cube format

Atomic coordinates and grid points in the reference frame given in the input

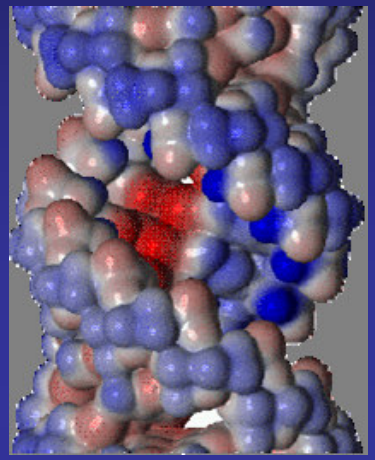
Reference frame orthogonal

Summary of different tools for post-processing and visualization

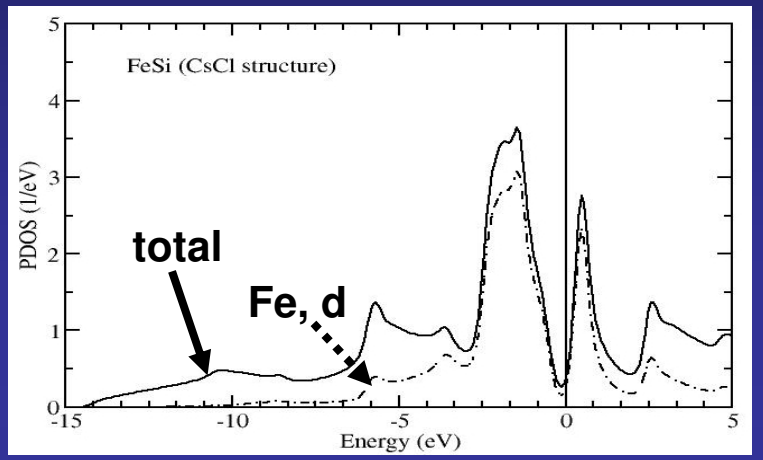
DENCHAR



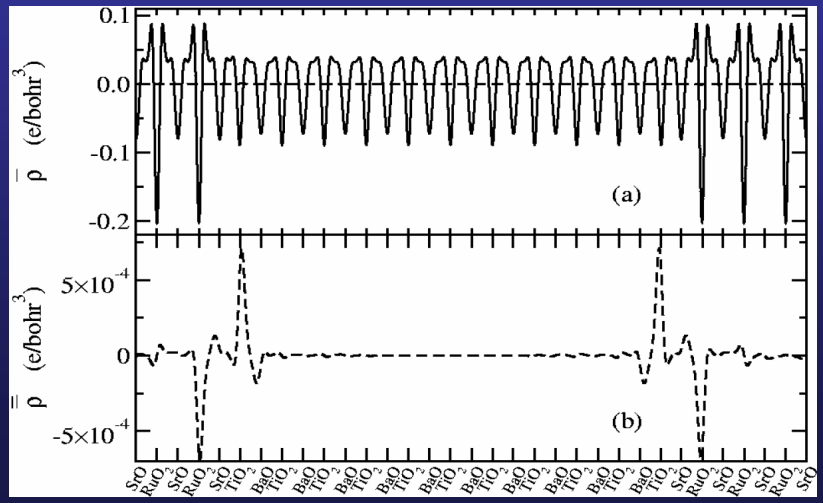
PLRHO



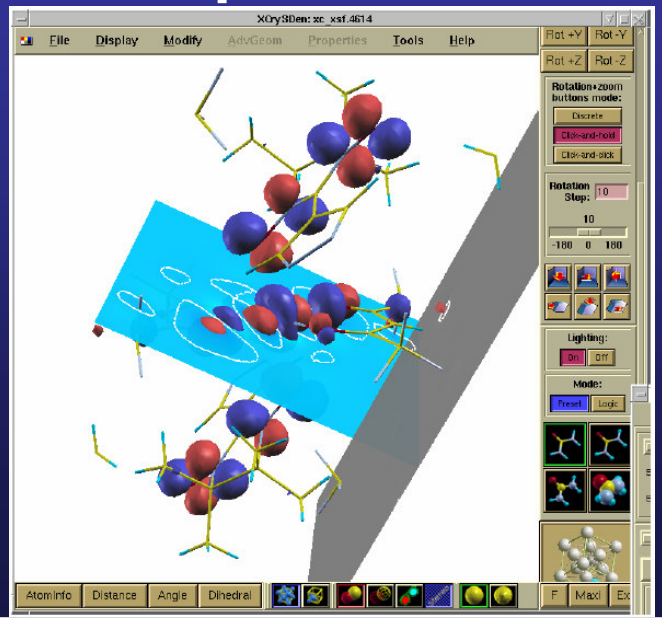
DOS, PDOS



MACROAVE



SIESTA's output with XCRYSDEN



PLRHO plots a 3D isosurface of the charge density and colours it with a second function

- $\rho(\vec{r})$
- LDOS integrated in a given energy interval
- $\rho(\vec{r})$ + electrostatic potential
- $\rho(\vec{r})$ + total potential
- $\rho(\vec{r})$ + spin density

Plrho reads the values of the functions in the real space grid and Interpolates to plot the 3D surface.

How to compile PLRHO

- First you need to install the PGPLOT library, available from

  http://www.astro.caltech.edu/~tjp/pgplot

- You can find plrho at

  ~/siesta/Utils/Plrho

- Then compile PLRHO with

  $ f90 plrho.f –lX11 –lpgplot –o plrho

- Check plrho_guide.txt for extra information.

How to run PLRHO

SIESTA

```
SaveRho                                .true.
SaveElectrostaticPotential             .true.
SaveTotalPotential                     .true.
%block LocalDensityOfStates
%block AtomicCoordinatesOrigin
```

Depending on what you want to plot

If you want to center the system

Output of SIESTA required by PLRHO

SystemLabel.RHO
SystemLabel.VH
SystemLabel.VT
SystemLabel.LDOS

PLRHO

Prepare the input file plrho.dat
$ plrho

You do not need to rerun SIESTA to run PLRHO as many times as you want

Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12    Saturation range for color function
 'unformatted'         Data format ('formatted'|'unformatted')
 '/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12    Saturation range for color function
 'unformatted'         Data format ('formatted'|'unformatted')
 '/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

'rho' $\rho(\vec{r})$

'ldos' LDOS integrated in a given energy interval

'vh' $\rho(\vec{r})$ + electrostatic potential

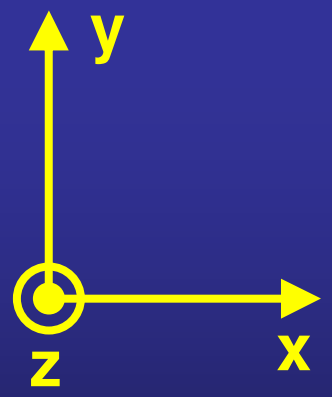
'vt' $\rho(\vec{r})$ + total potential

'spin' $\rho(\vec{r})$ + spin density

Input of PLRHO: plrho.dat

```
  'h2o'                 System label, used to name input files
  'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
  90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
  4.e-3                 Value of electron density (or LDOS) for isosurface
 -0.08  +0.01  +0.12 Saturation range for color function
  'unformatted'         Data format ('formatted'|'unformatted')
  '/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Viewpoint is always from above (positive z axis)

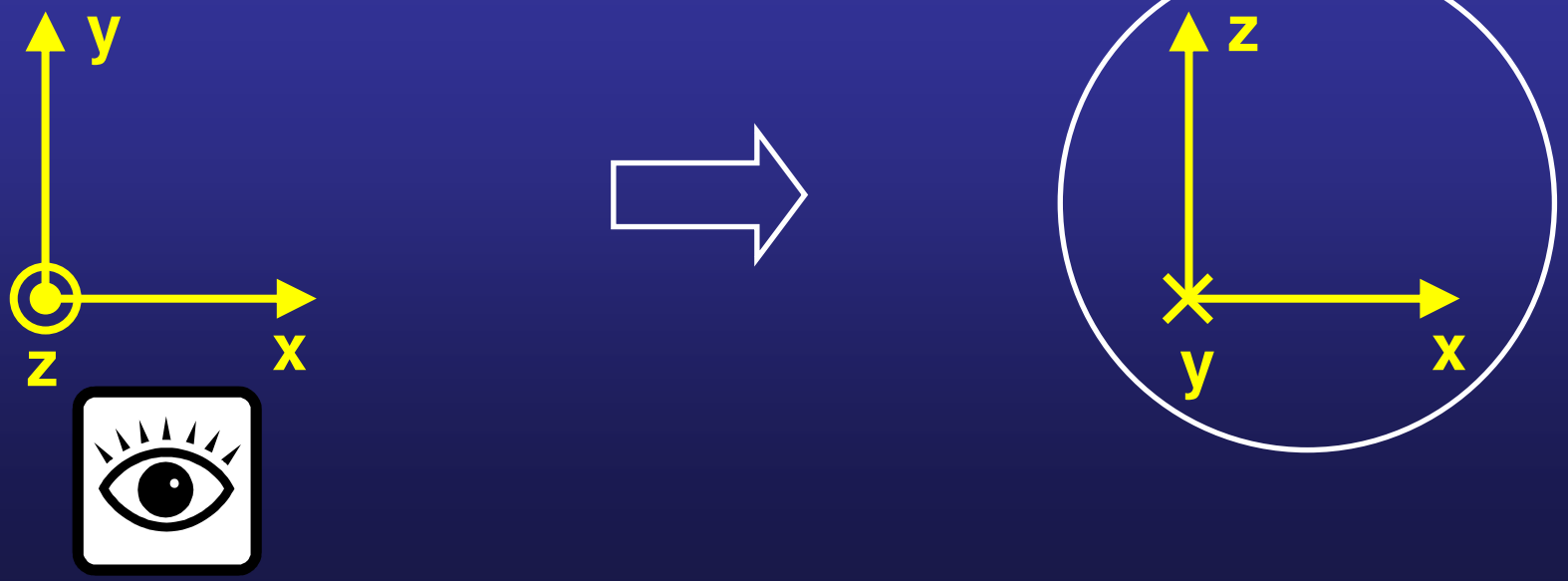


To view the system from a different angle, rotate it with the Euler angles

Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12 Saturation range for color function
 'unformatted'         Data format ('formatted'|'unformatted')
 '/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Example: view from –y (Euler angles = 90 -90 -90)

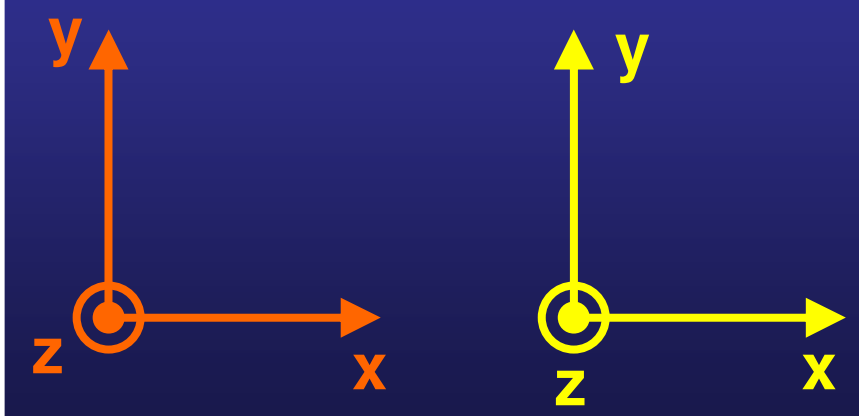


Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12 Saturation range for color function
 'unformatted'        Data format ('formatted'|'unformatted')
 '/CPS'              Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Example: view from –y (Euler angles = 90 -90 -90)

Reference axes **System axes**



Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12 Saturation range for color function
 'unformatted'         Data format ('formatted'|'unformatted')
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```
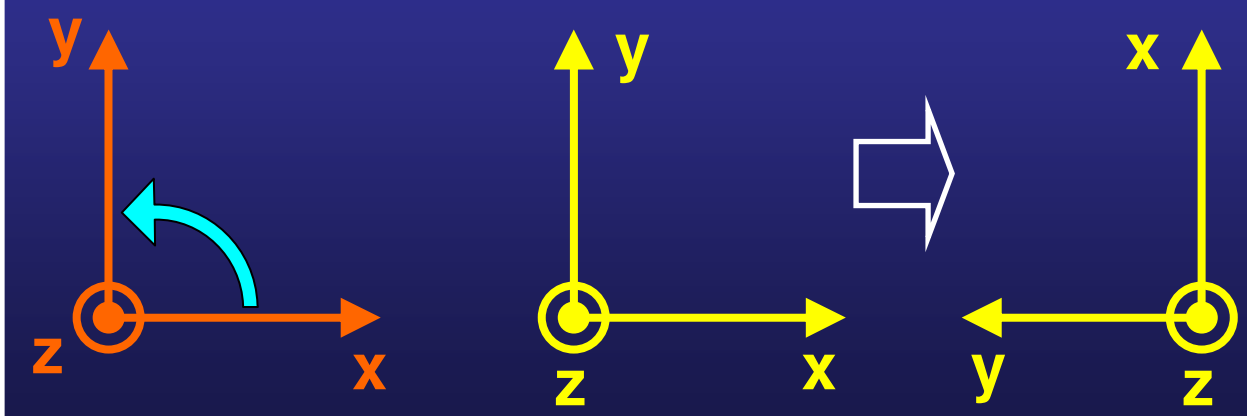

Example: view from –y (Euler angles = 90 -90 -90)

Reference axes **System axes**



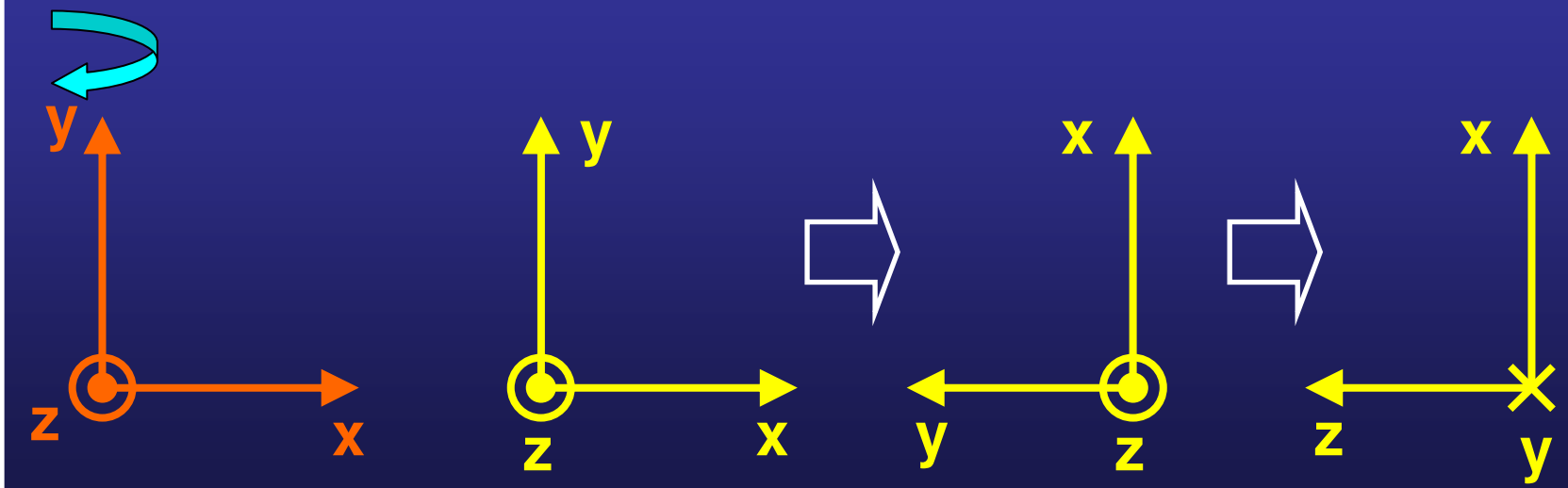
Alpha: first rotation around z

Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12 Saturation range for color function
 'unformatted'         Data format ('formatted'|'unformatted')
 '/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Example: view from –y (Euler angles = 90 -90 -90)

Reference axes **System axes**



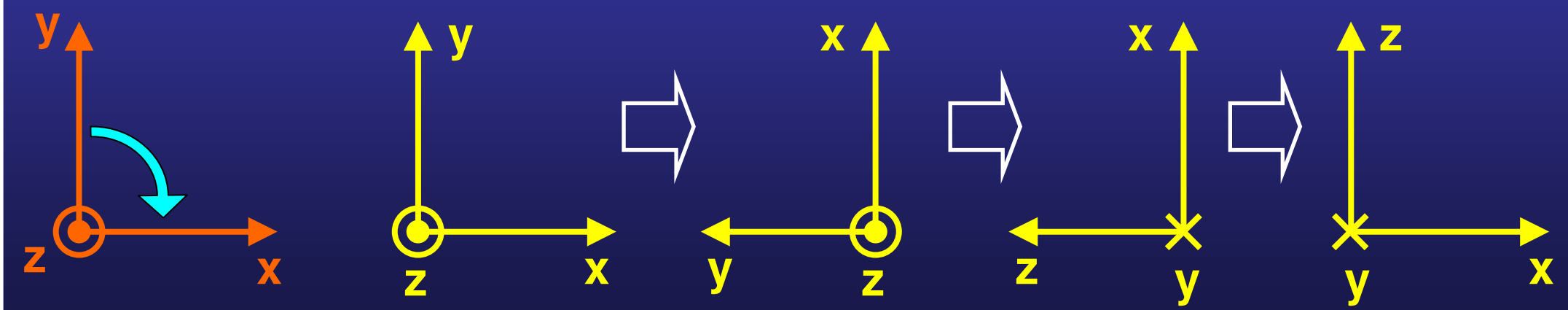
Beta: rotation around y

Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
 'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
 4.e-3                 Value of electron density (or LDOS) for isosurface
-0.08  +0.01  +0.12 Saturation range for color function
 'unformatted'        Data format ('formatted'|'unformatted')
 '/CPS'              Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Example: view from –y (Euler angles = 90 -90 -90)

Reference axes **System axes**



Input of PLRHO: plrho.dat

```
 'h2o'                 System label, used to name input files
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'unformatted'         Data format ('formatted'|'unformatted')
'/CPS'               Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

Value of colouring function

Potential or Spin

Third value: maximum saturation range — **blue**

Second value: mean saturation range — **white**

First value: minimum saturation range — **red**

Pure blue

Interpolation white/blue

Interpolation red/white

Pure red

Output of PLRHO

```
  'h2o'                 System label, used to name input files
  'vh'                  Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
  90.0  0.0  -90.0      Euler rotation angles alpha, beta, gamma
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  'unformatted'         Data format ('formatted'|'unformatted')
  '/CPS'              Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```

screen grey-scale postscrip colour postscrip

Output of PLRHO

```
 'h2o'                System label, used to name input files
 'vh'                 Function(s) to plot ('rho'|'ldos'|'spin'|'vt'|'vh')
 90.0  0.0  -90.0     Euler rotation angles alpha, beta, gamma
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 'unformatted'        Data format ('formatted'|'unformatted')
 '/CPS'              Output option ('/XWIN'|'/PS'|'/CPS'|+more)
```
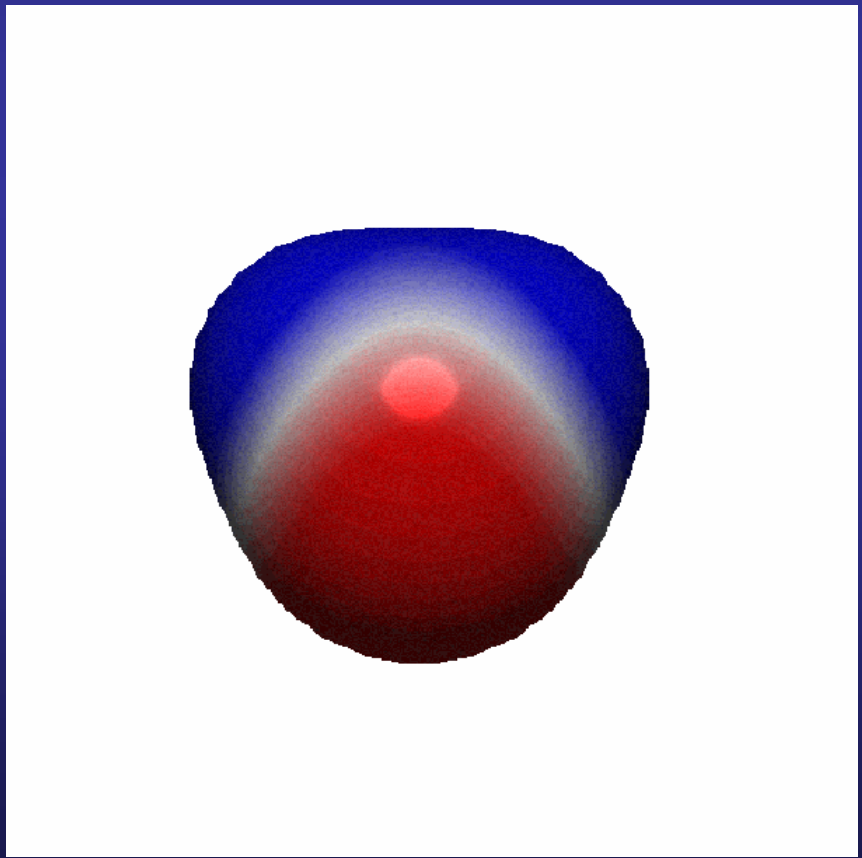
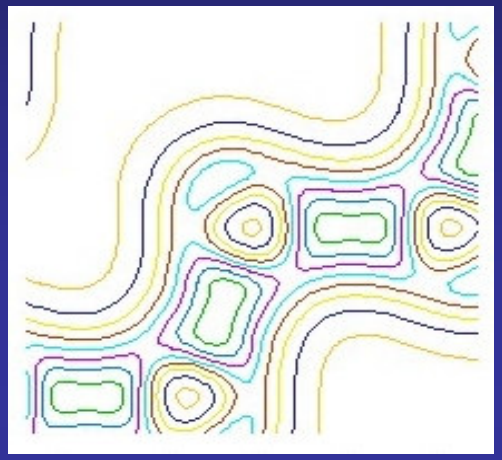

H_2O molecule

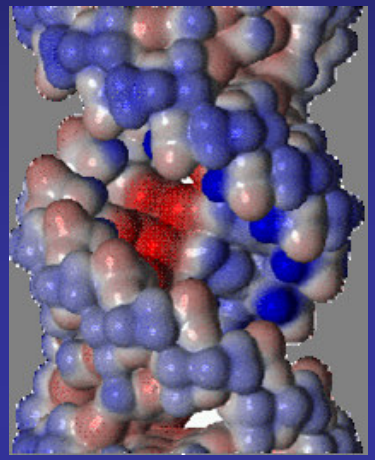


Summary of different tools for post-processing and visualization

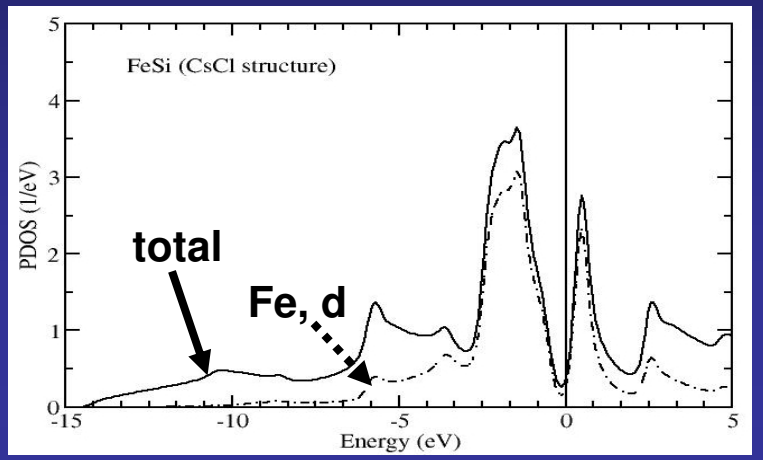
DENCHAR



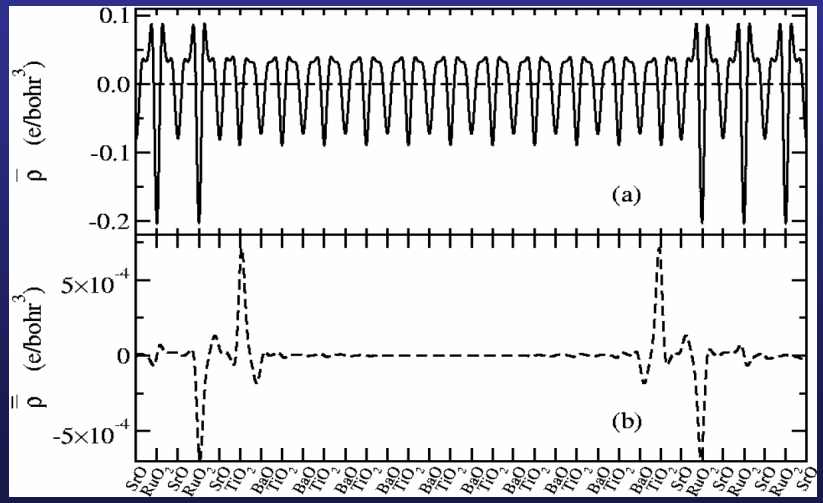
PLRHO



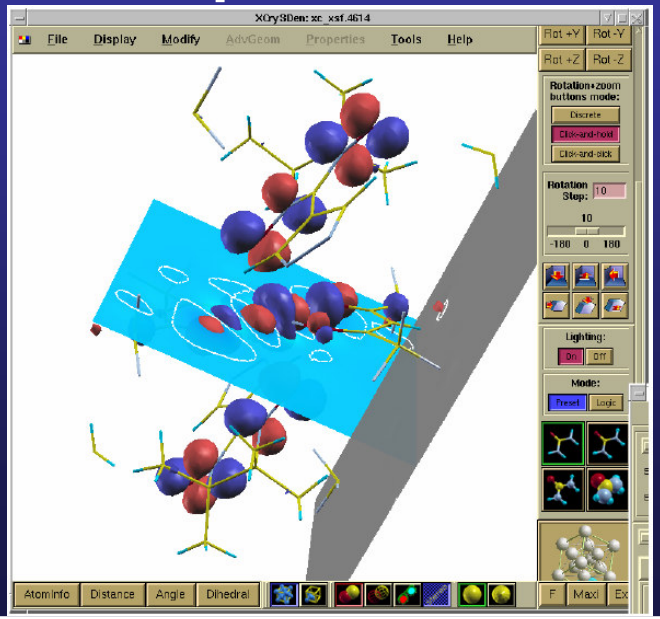
DOS, PDOS



MACROAVE



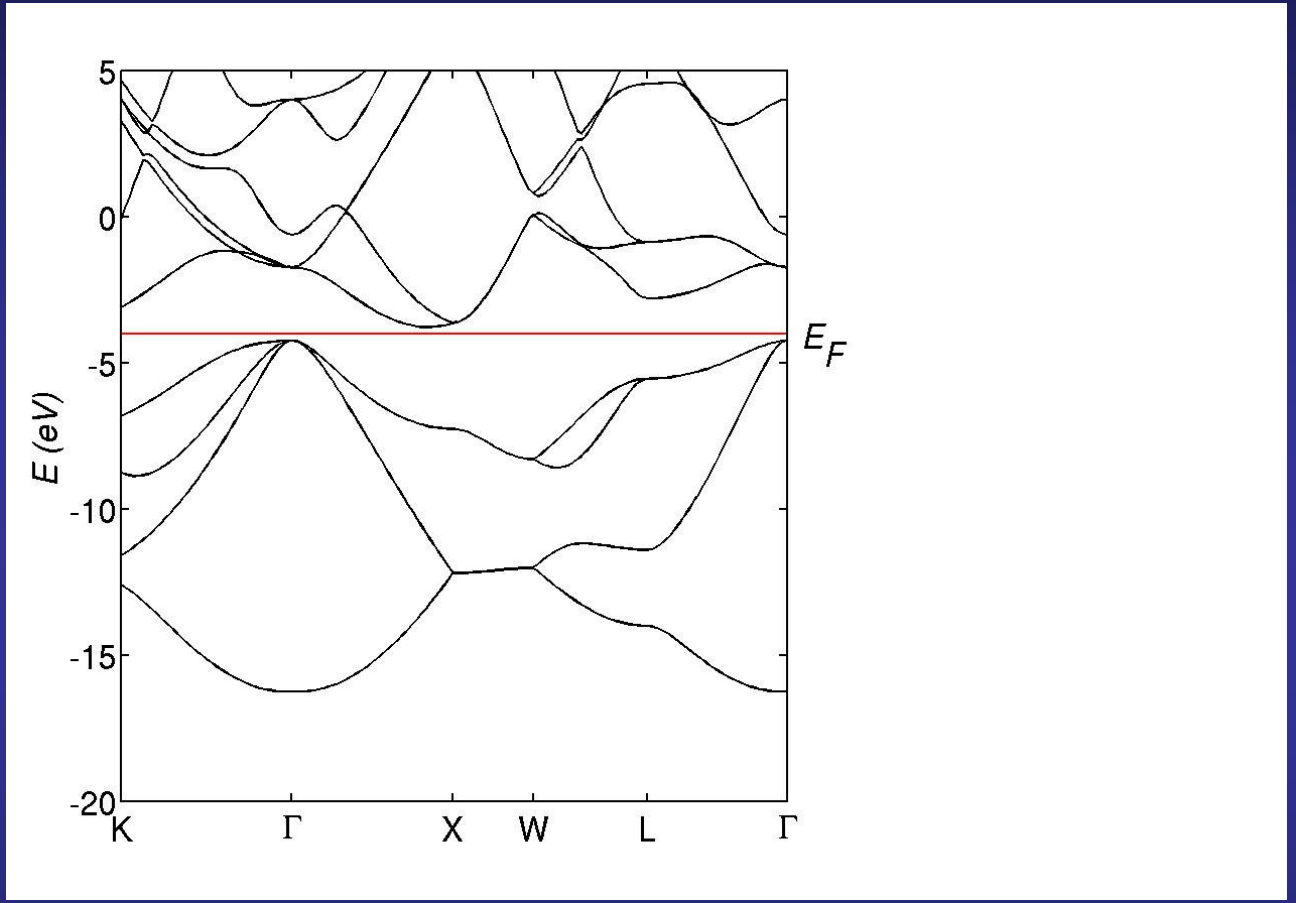
SIESTA's output with XCRYSDEN



Density Of States (DOS)

$g(E)dE$ **the number of one-electron levels between** E **and** $E + dE$

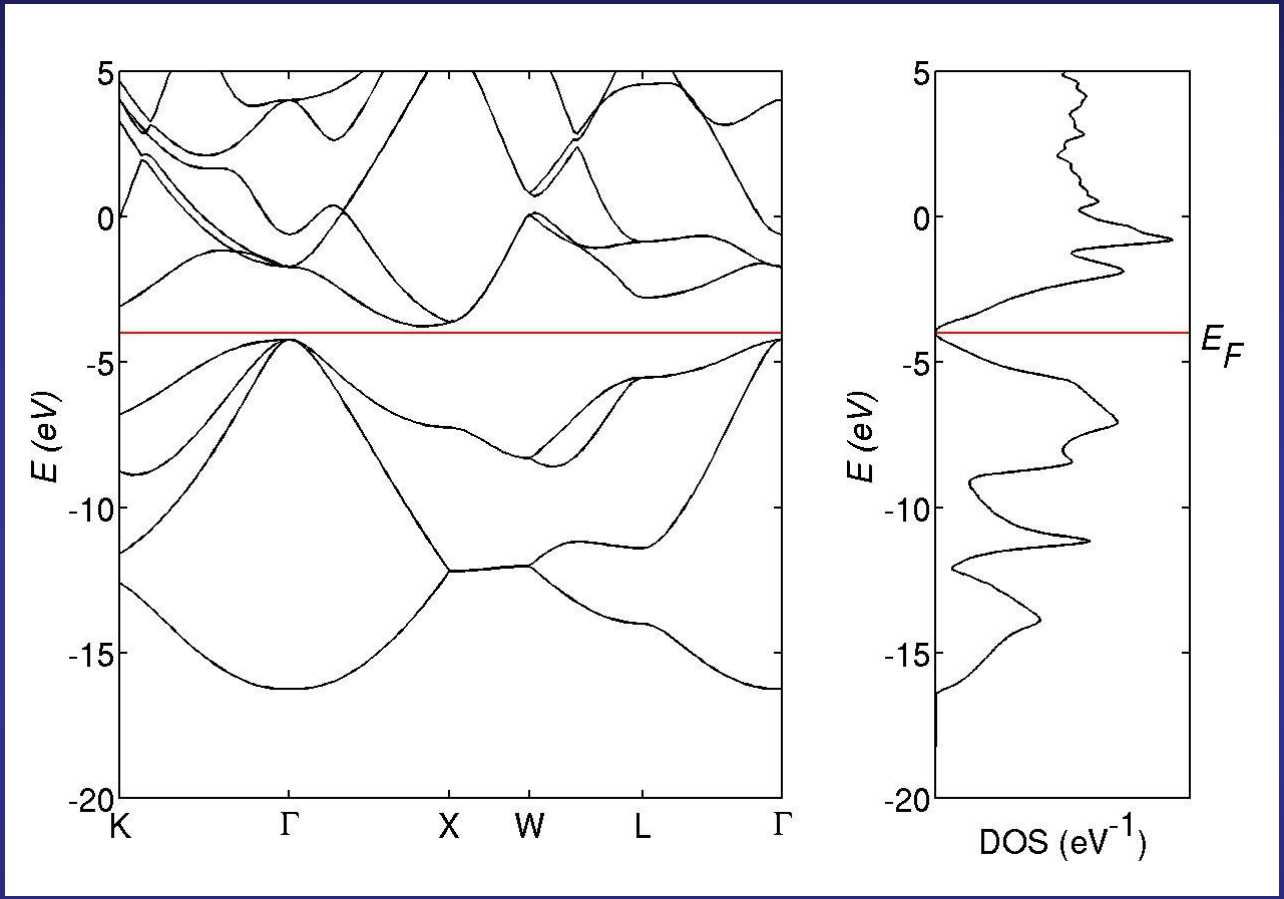
Si bulk



Density Of States (DOS)

$g(E)dE$ **the number of one-electron levels between** E **and** $E + dE$

Si bulk



$$g(E) = \frac{1}{N_{\vec{k}}} \sum_{i}^{bands} \sum_{\vec{k}} \delta\left(E - E_i(\vec{k})\right)$$

Units: (Energy)$^{-1}$

Projected Density Of States (PDOS)

$g_\mu(E)dE$ the number of one-electron levels with weight on orbital μ between E and $E + dE$

$$g_\mu(E) = \frac{1}{N_{\vec{k}}} \sum_{i}^{bands} \sum_{\vec{k}} \sum_{\nu} c^*_{\nu i}(\vec{k}) c_{\mu i}(\vec{k}) S_{\nu\mu}(\vec{k}) \delta\left(E - E_i(\vec{k})\right)$$

Coefficients of the eigenvector $\psi_i(\vec{k})$ with eigenvalue $E_i(\vec{k})$

Overlap matrix of the atomic basis

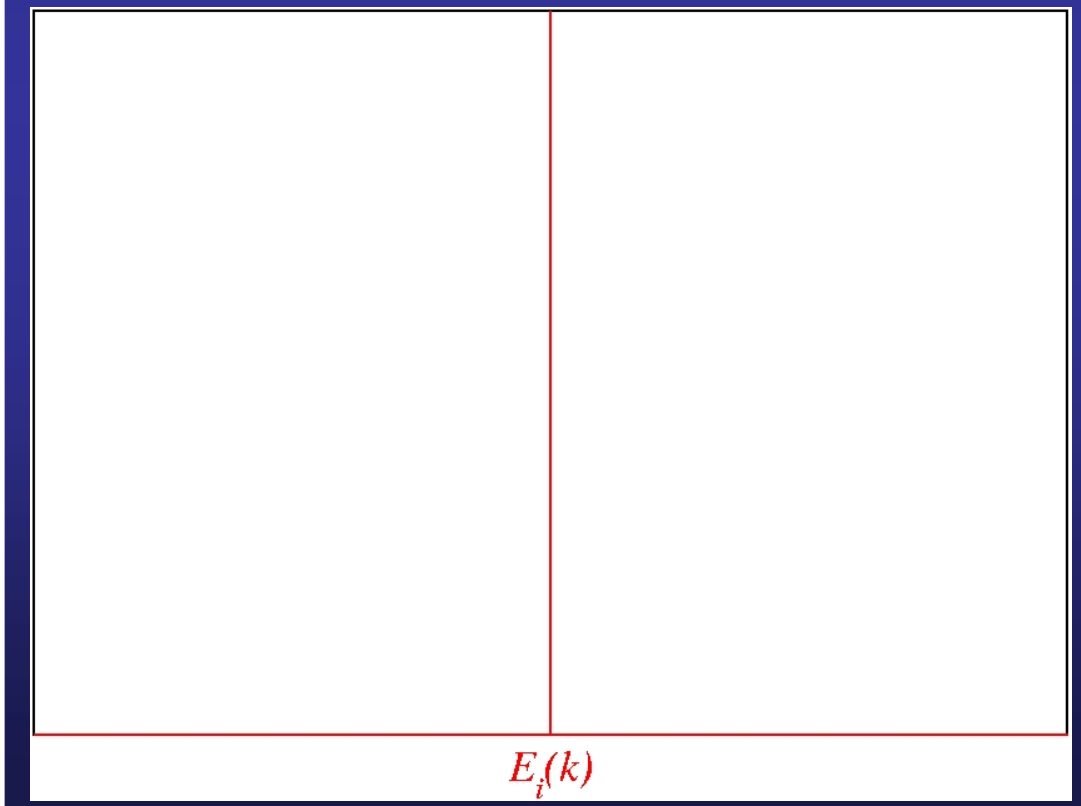
Units: $(\text{Energy})^{-1}$

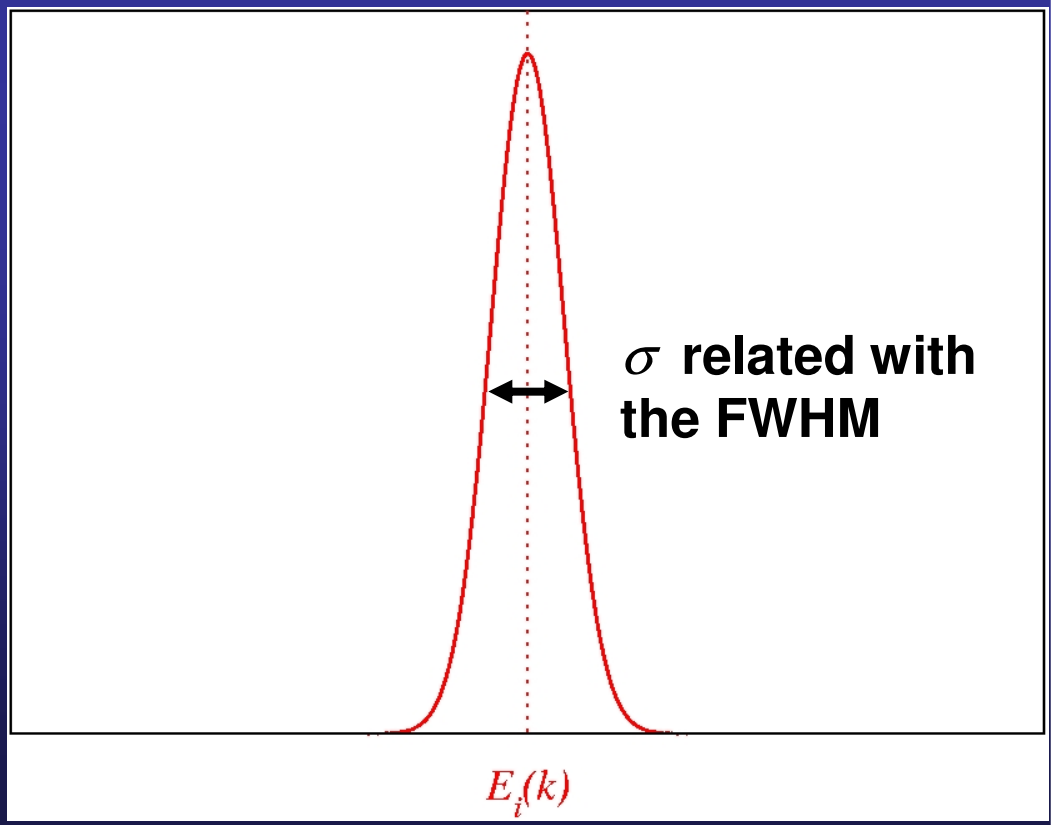
Relation between the DOS and PDOS:

$$g(E) = \sum_{\mu} g_\mu(E)$$

The eigenvalues are broadening by a gaussian to smooth the shape of the DOS and PDOS

$$\delta\left(E - E_i(\vec{k})\right) \rightarrow \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{\left(E - E_i(\vec{k})\right)^2}{\sigma^2}}$$





Two step procedure to produce smooth DOS and PDOS

First:

Run a simulation with a sensible (converged) number of k-points

kgrid_cutoff

%block kgrid_Monkhorst_Pack

Get converged geometry and density matrix

Second:

Starting from the previously converged geometry and density matrix, run a single SCF step with fixed geometry, with many more k-points

DM.UseSaveDM	.true.
MaxSCFIterations	1
MD.NumCGsteps (or equivalent)	0

Increase number of k-points (see above)

%block ProjectedDensityOfStates

How to compute the DOS and PDOS

```
%block ProjectedDensityOfStates
     -20.0  10.0  0.200 500 eV
%endblock ProjectedDensityOfStates
```

-20.0 10.0 : Energy window where the DOS and PDOS will be computed

How to compute the DOS and PDOS

```
%block ProjectedDensityOfStates
     -20.0  10.0  0.200 500 eV
%endblock ProjectedDensityOfStates
```

-20.0 10.0 : Energy window where the DOS and PDOS will be computed

0.200 : Peak width of the gaussian used to broad the eigenvalues (energy)

How to compute the DOS and PDOS

```
%block ProjectedDensityOfStates
     -20.0  10.0  0.200 500 eV
%endblock ProjectedDensityOfStates
```

-20.0 10.0 : Energy window where the DOS and PDOS will be computed

0.200 : Peak width of the gaussian used to broad the eigenvalues (energy)

500 : Number of points in the histogram

How to compute the DOS and PDOS

```
%block ProjectedDensityOfStates
     -20.0  10.0  0.200 500 eV
%endblock ProjectedDensityOfStates
```

-20.0 10.0 : Energy window where the DOS and PDOS will be computed

0.200 : Peak width of the gaussian used to broad the eigenvalues (energy)

500 : Number of points in the histogram

eV : Units in which the previous energies are introduced

Output for the Density Of States

SystemLabel.DOS

Format

Energy (eV)	DOS Spin Up (eV^{-1})	DOS Spin Down (eV^{-1})
-15.99598	0.03075	0.00000
-15.97596	0.03580	0.00000
-15.95594	0.04115	0.00000
.	.	.
.	.	.

Output for the Projected Density Of States

SystemLabel.PDOS

```
<pdos>
<nspin>1</nspin>
<norbitals>  26</norbitals>
<energy_values units="eV">
           -19.99998
           -19.97996
           -19.95994
                .
                .
                .
</energy_values>
<orbital
 index="1"
 atom_index="1"
 species="Si"
 position="   0.000000   0.000000   0.000000"
 n="3"
 l=" 0"
 m=" 0"
 z="1"
>
<data>
   0.00000
   0.00000
   0.00000
       .
       .
       .
</data>
</orbital>
</pdos>
```

Written in XML

Energy Window

One element <orbital> for every atomic orbital in the basis set

How to digest the SystemLabel.PDOS file

During the compilation of SIESTA

For some compilers, the libwxml.a library needs to be compiled with
"-DWXML_INIT_FIX"
(see known issues in http://fisica.ehu.es/ag/siesta-extra/issues.html)

pdosxml (by Alberto García)

Siesta/Util/pdosxml

Edit the readme file to:

Learn how to select the orbitals whose PDOS will be accumulated

How to compile the code

How to run the code

fmpdos (by Andrei Postnikov)

Download from

http://www.home.uni-osnabrueck.de/apostnik/download.html

Compile and follow the instructions at run-time

Normalization of the DOS and PDOS

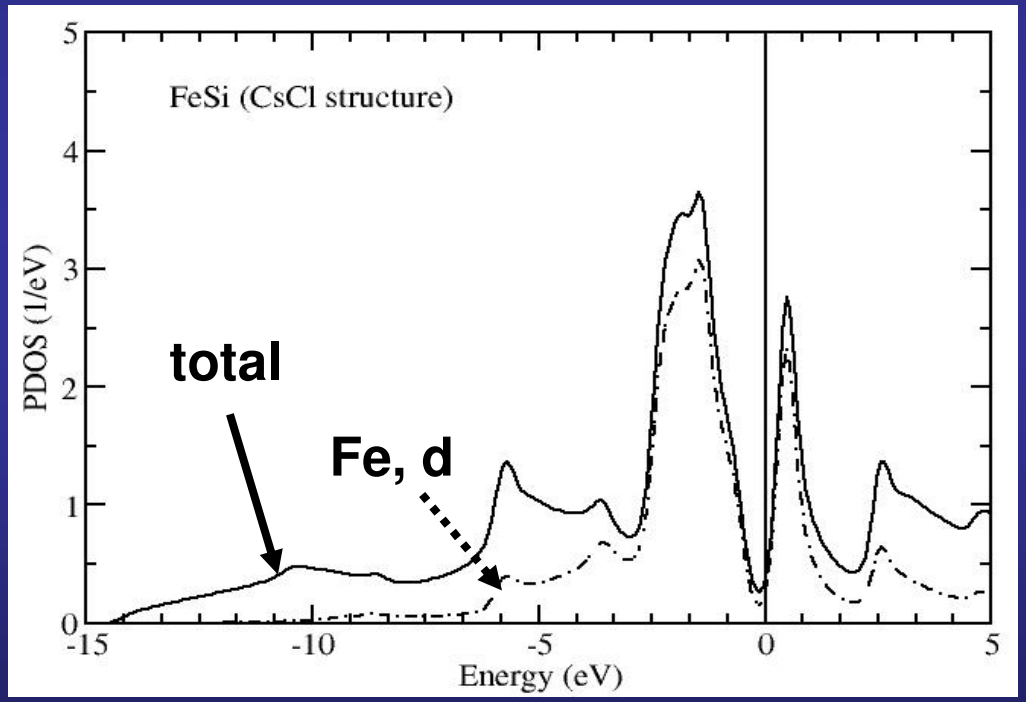
$$\int_{-\infty}^{+\infty} g(E)\, dE =$$ Number of bands per k-point $=$ Number of atomic orbitals in the unit cell

$$\int_{-\infty}^{+\infty} g(E)n(E)\, dE =$$ Number of electrons in the unit cell

Occupation factor at energy E

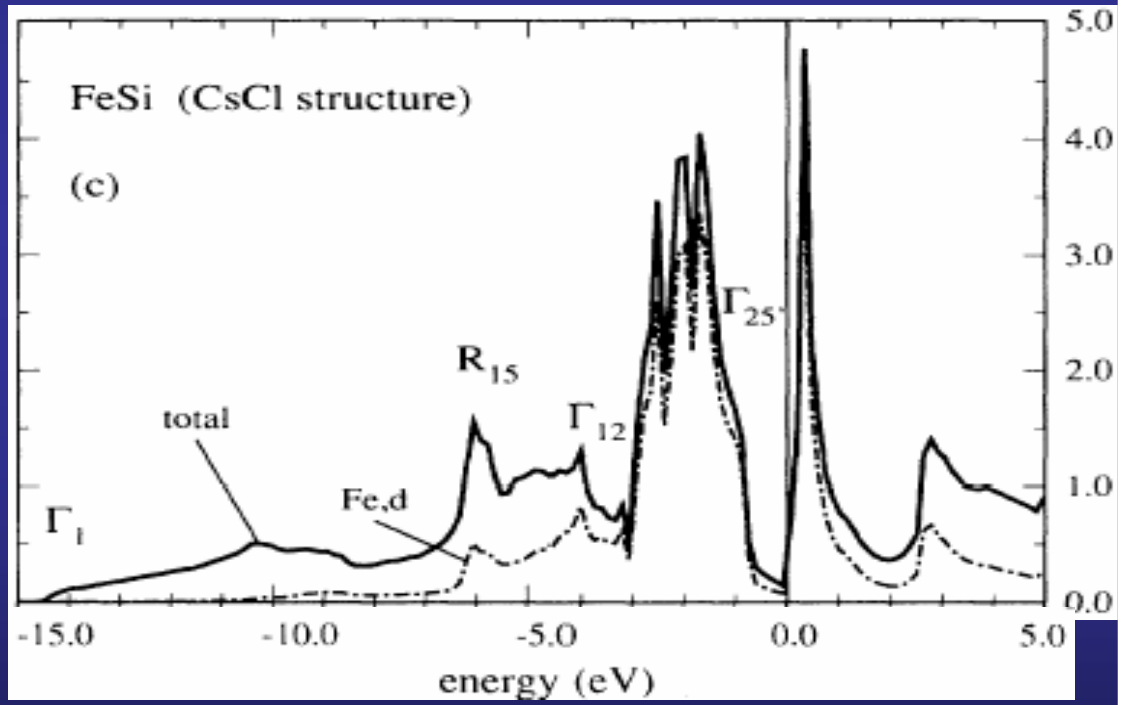
Example of DOS and PDOS

$$g_\mu(E) = \frac{1}{N_{\vec{k}}} \sum_{i}^{bands} \sum_{\vec{k}} \sum_{\nu} c^*_{\nu i}(\vec{k}) c_{\mu i}(\vec{k}) S_{\nu\mu}(\vec{k}) \delta\left(E - E_i(\vec{k})\right)$$



J. Junquera *et al.* Surf. Sci. 482-485, 625 (2001)

SIESTA, single-zeta polarized basis

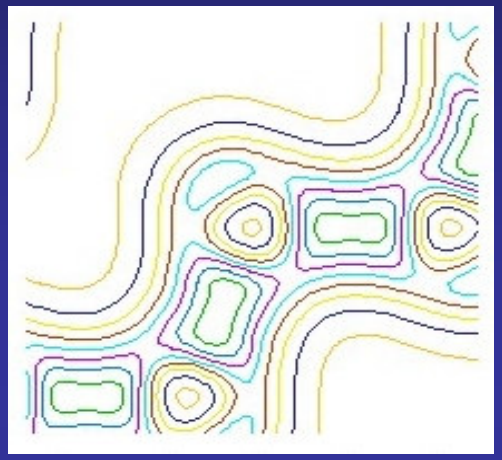


K. A. Mäder *et al.* Phys. Rev. B 48, 4364 (1998)

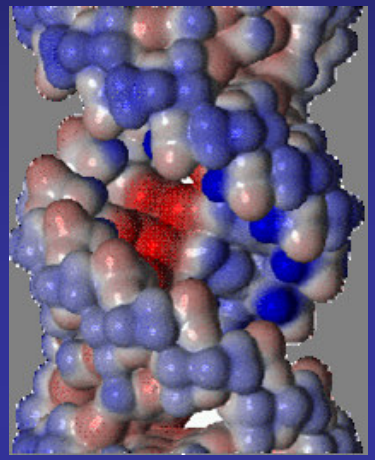
All electron calculation

Summary of different tools for post-processing and visualization

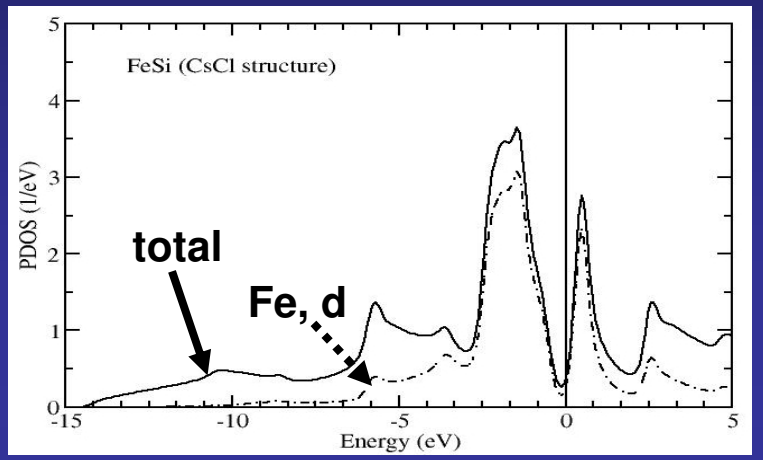
DENCHAR



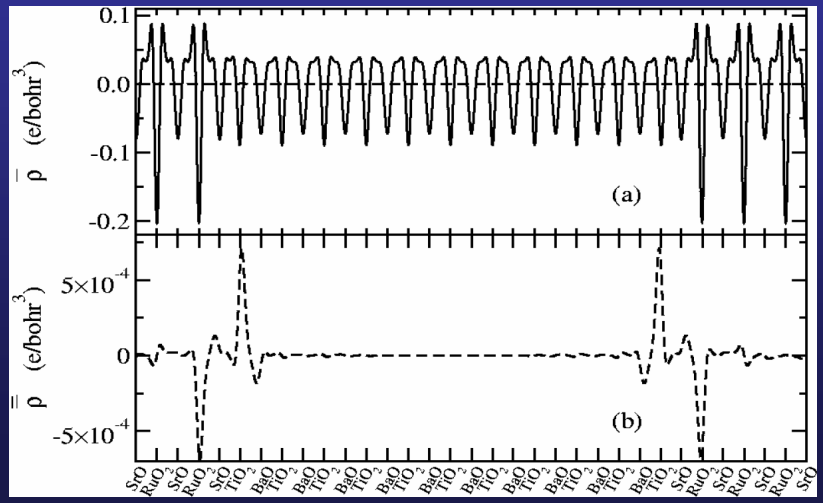
PLRHO



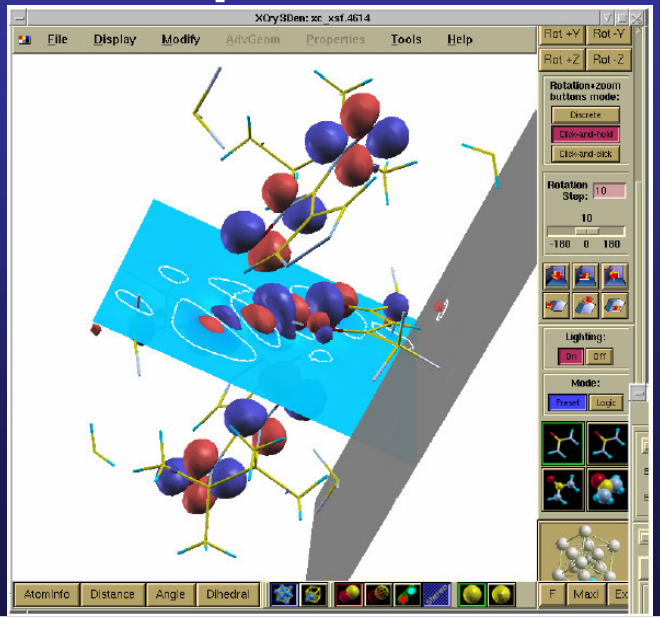
DOS, PDOS



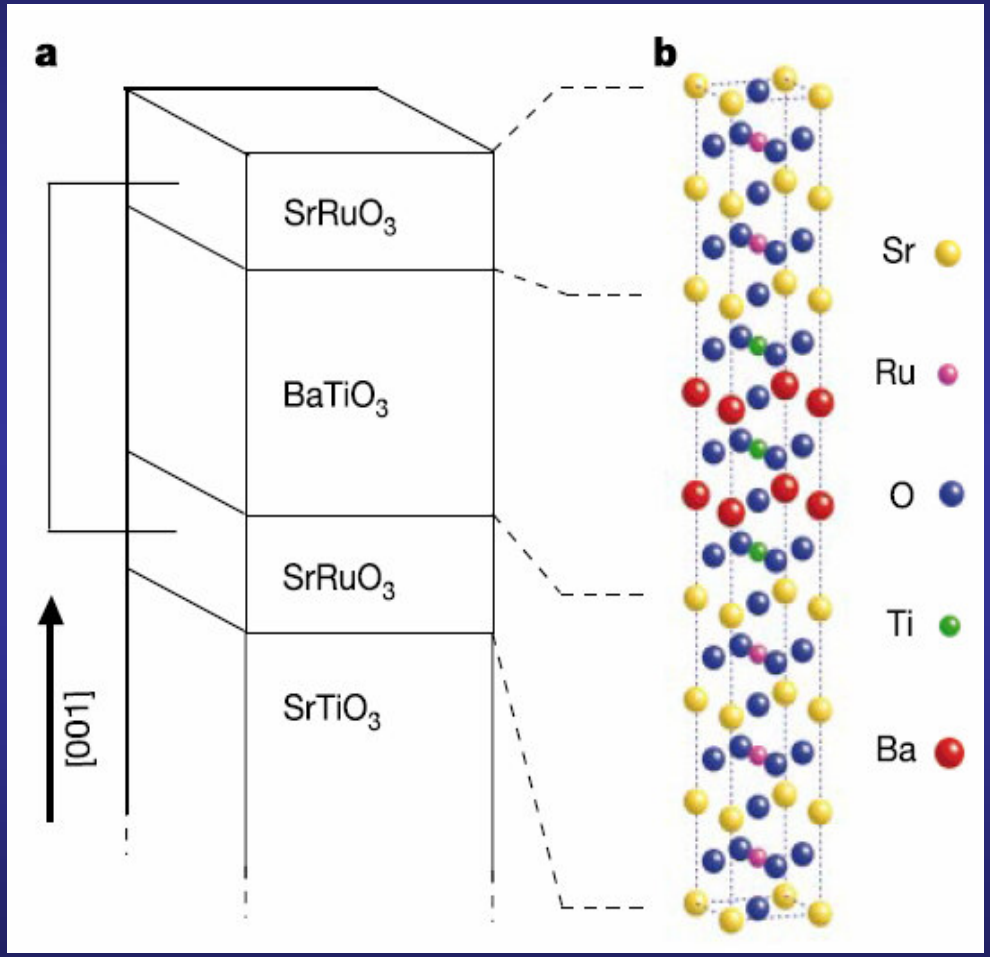
MACROAVE

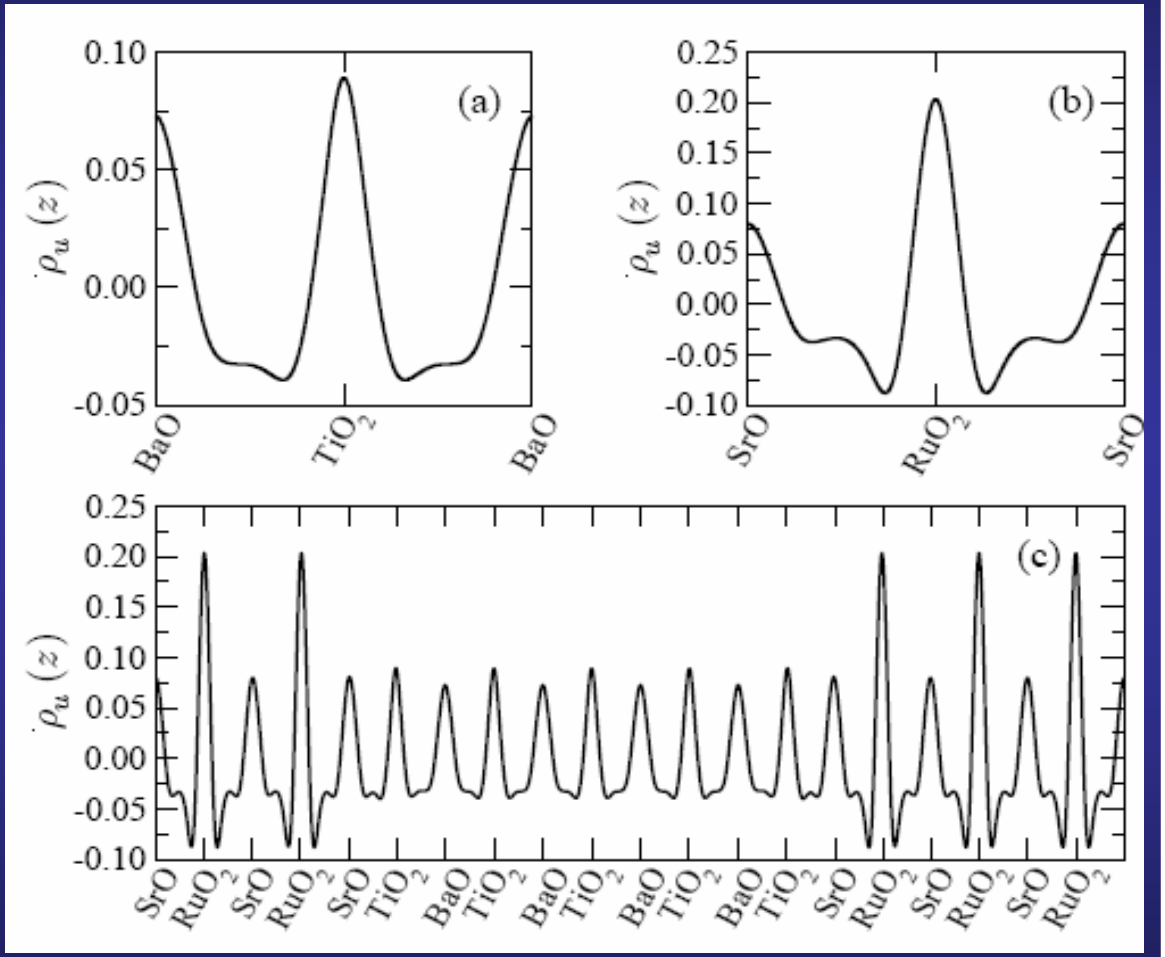


SIESTA's output with XCRYSDEN



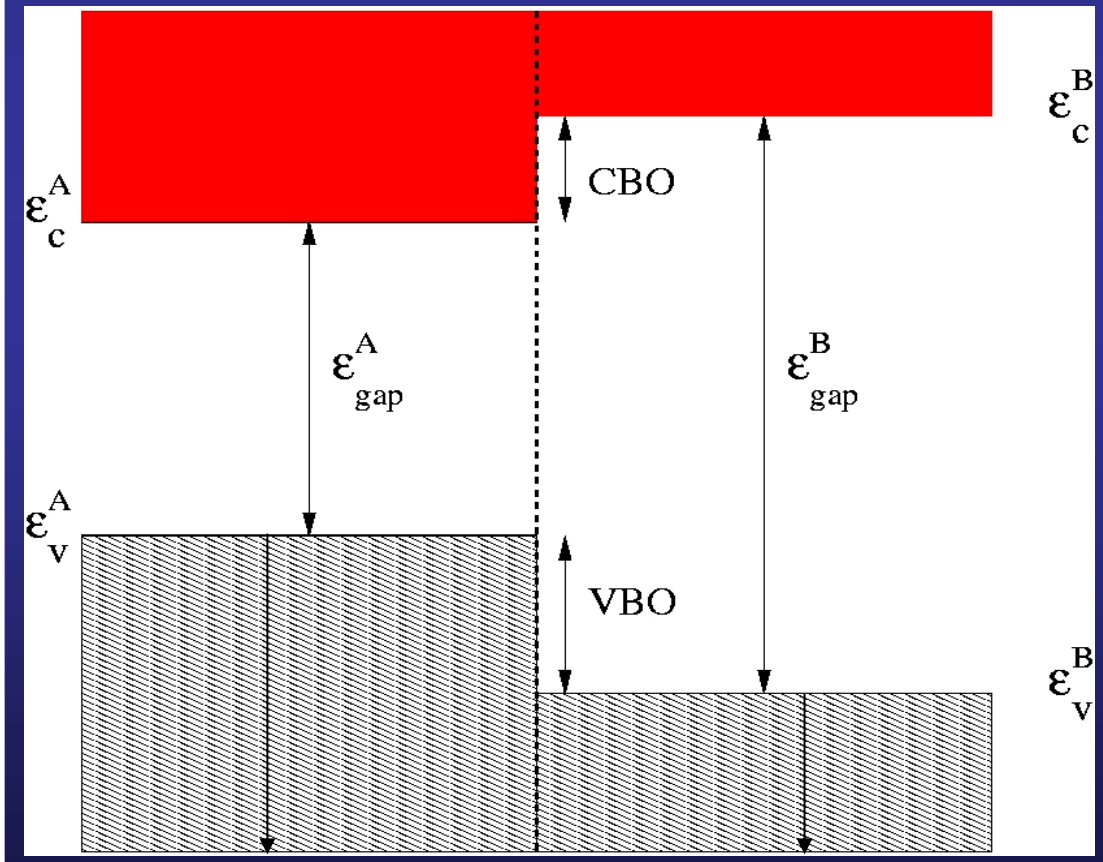
How to extract from the immense detail provided by first-principles calculations on surfaces reliable values of the physical quantities of interest





Physical quantities of interest in surfaces and interfaces

- Charge densities at the surface/interface
- Dipole moment densities at the surface/interface
- Work functions (surfaces) and band offsets (interfaces)



$$VBO = \Delta E_v + \Delta V$$

ΔE_v : the band structure term

Difference of the top of the valence bands

From two independent bulk band structure calculations of the bulk material

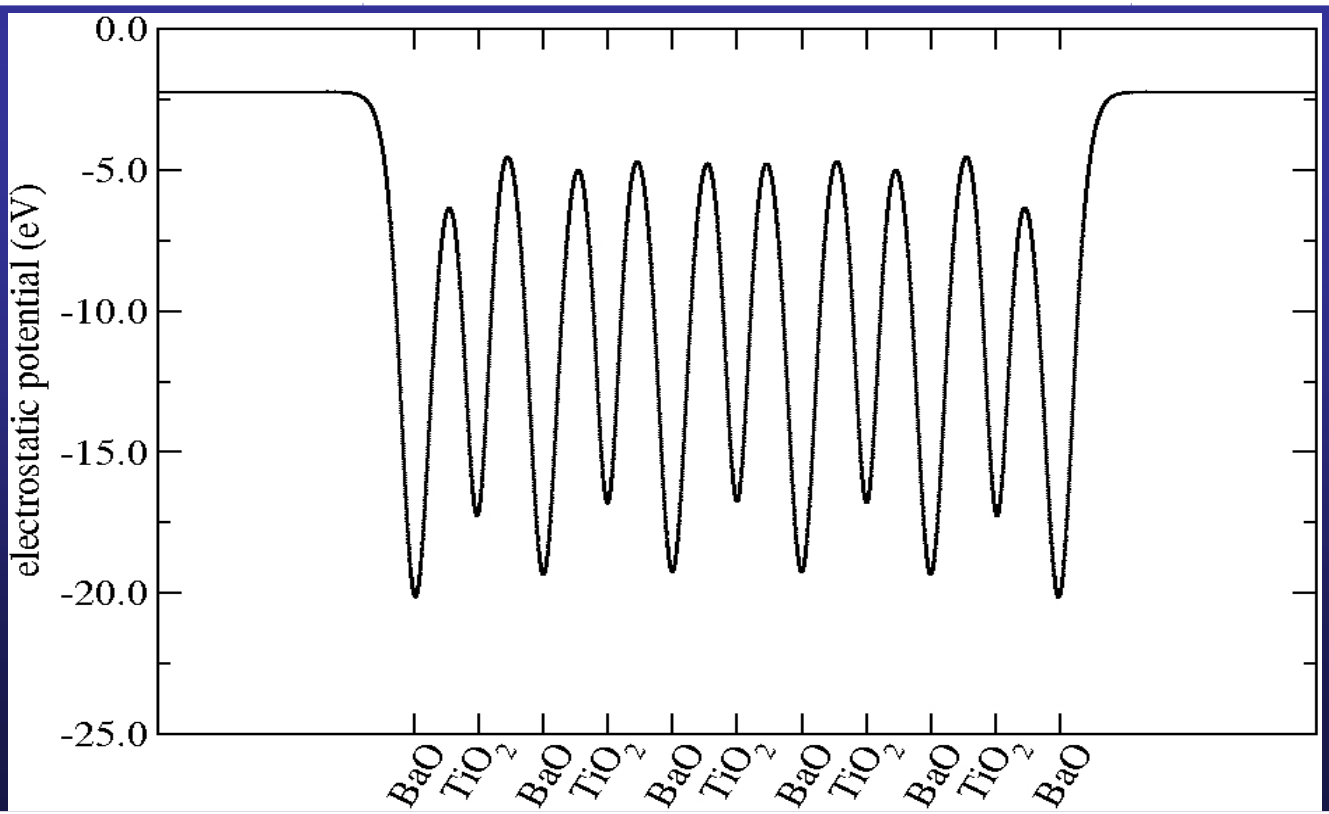
ΔV : jump of the average electrostatic potential

Contains all the intrinsic interface effects

Obtained by nanosmoothing the electrostatic potential

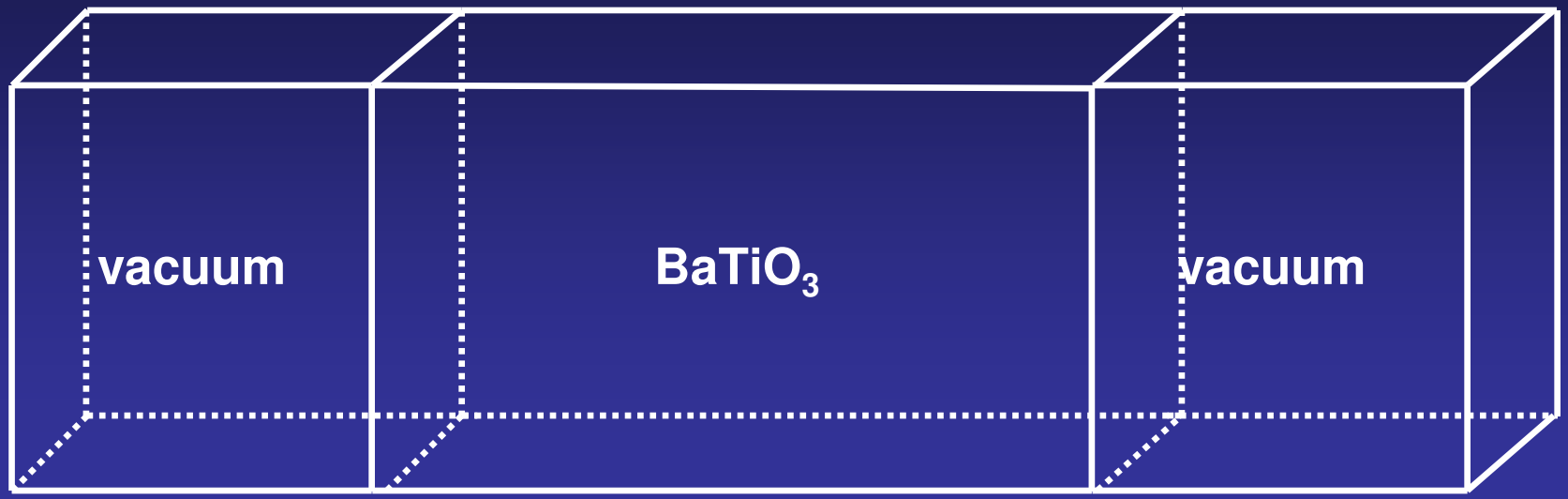
First step: average in the plane

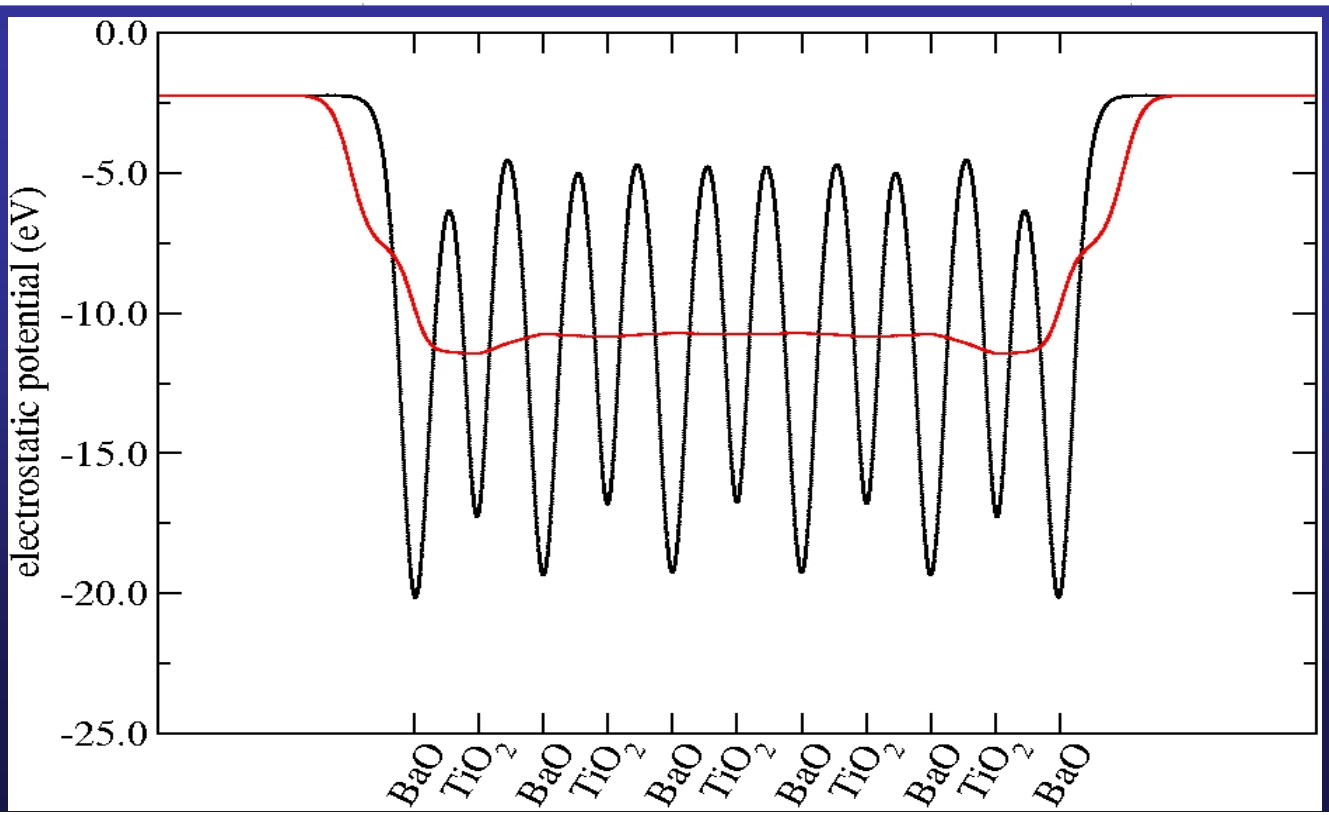
$$\overline{V}(z) = \frac{1}{S}\int_S dxdy\ V(\vec{r})$$



Second step: nanosmooth the planar average on the z-direction

$$\overline{\overline{V}}(z) = \int dz' \; f(z - z')\overline{V}(z')$$

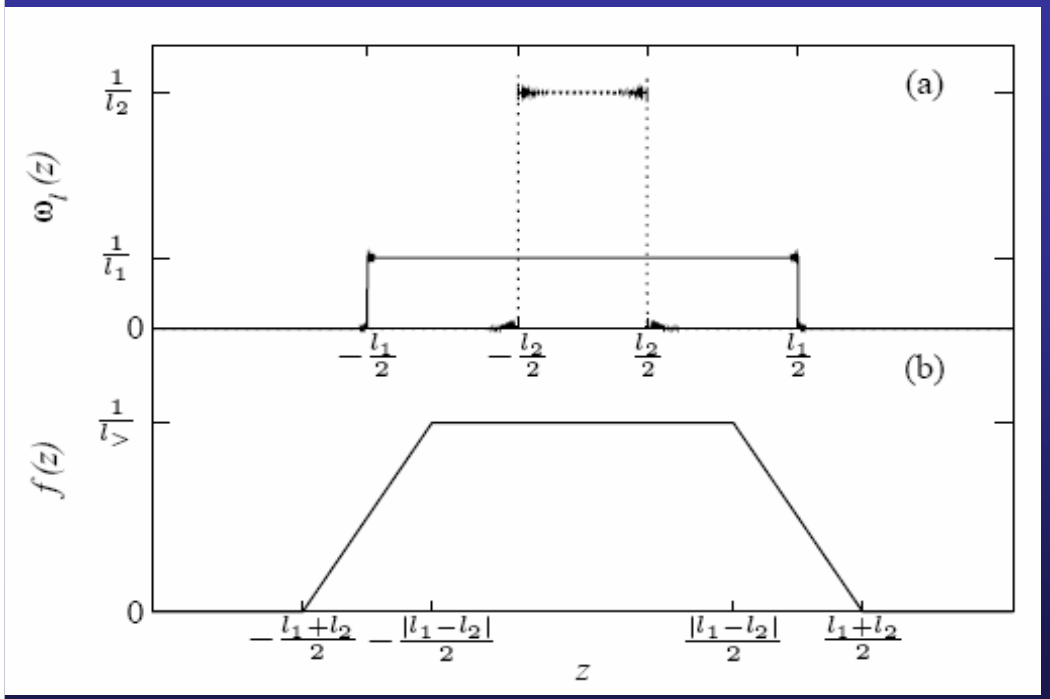


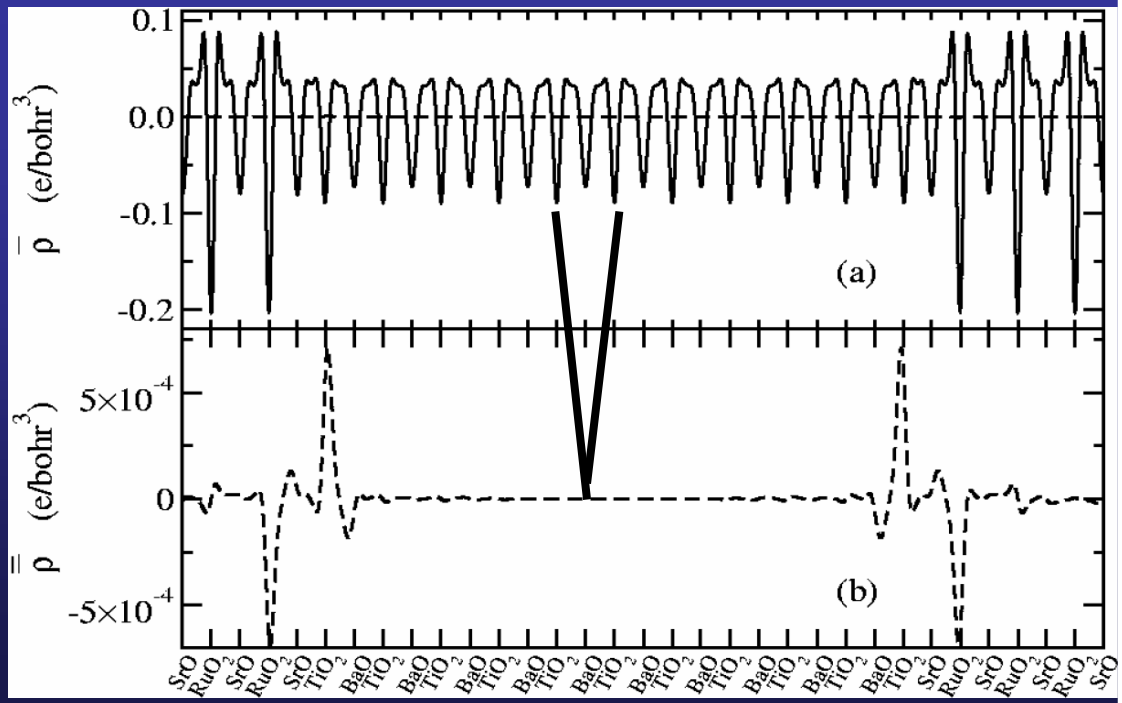


Atomic scale fluctuations are washed out by filtering the magnitudes via convolution with smooth functions

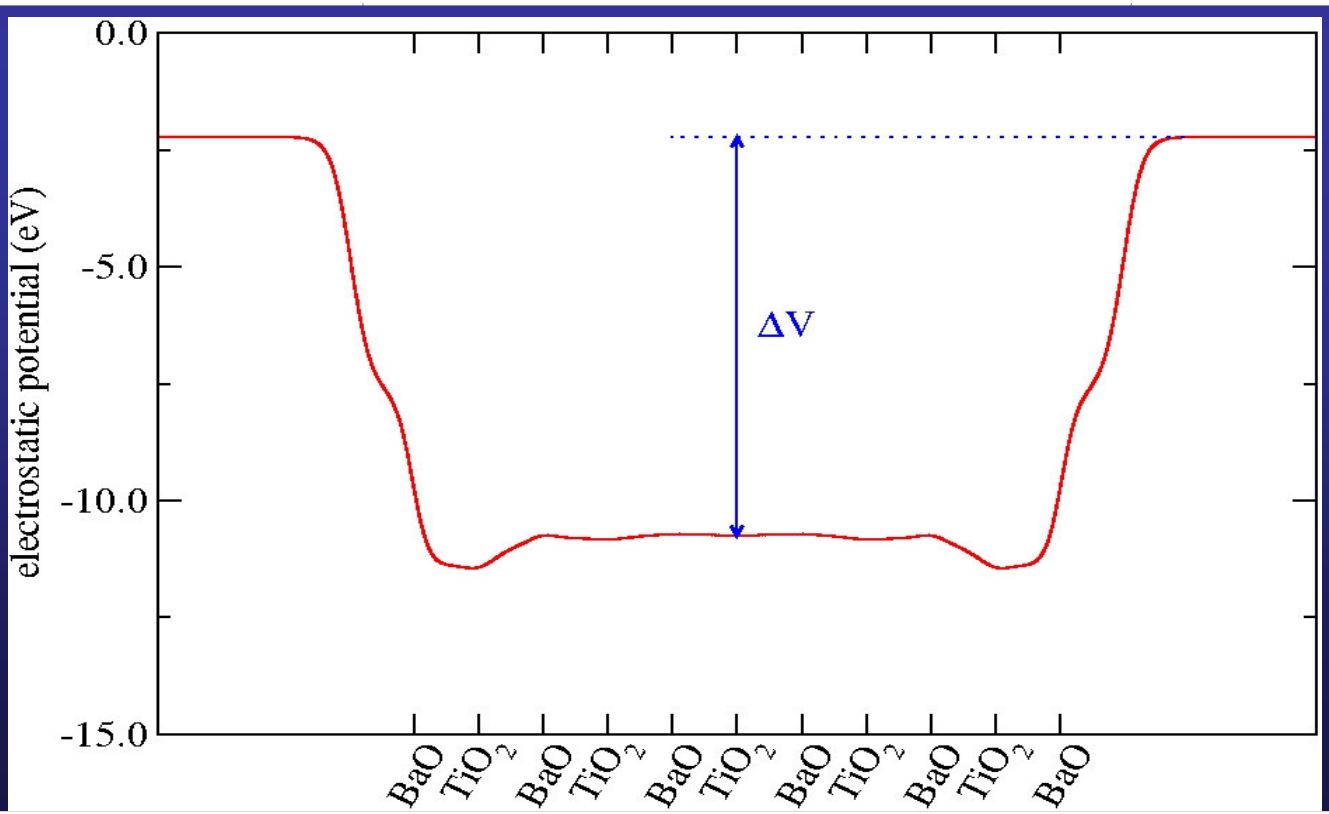
$$\overline{\overline{\rho}}(z) = \int dz' f(z - z')\bar{\rho}(z')$$

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





ΔV is readily obtained from the nanosmoothed potential



How to compile MACROAVE…

```
$ cd ~/siesta/Util/Macroave/Src/
$ make
ifort -c -O3  defs_basis.f90
ifort -c -O3  defs_common.f90
ifort -c -O3  io.f
ifort -c -O3  iorho.f
ifort -c -O3  paste.f
ifort -c -O3  macroave.f
ifort -c -O3  thetaft.f
ifort -c -O3  surpla.f
ifort -c -O3  volcel.f
ifort -c -O3  recipes.f
ifort -c -O3  hdr_io.f90
ifort -o macroave.x \
       defs_basis.o defs_common.o io.o iorho.o paste.o macroave.o thetaft.o
       surpla.o volcel.o recipes.o hdr_io.o
```

Use the **same arch.make** file as for the compilation of **serial SIESTA**

…and where to find the User's Guide and some Examples

```
$ cd ~/siesta/Util/Macroave
$ ls
Docs  Examples  Src
```

How to run MACROAVE

SIESTA

SaveRho	.true.
SaveTotalCharge	.true.
SaveIonicCharge	.true.
SaveDeltaRho	.true.
SaveElectrostaticPotential	.true.
SaveTotalPotential	.true.

Depending on what you want to nanosmooth

Output of SIESTA required by MACROAVE

SystemLabel.RHO
SystemLabel.TOCH
SystemLabel.IOCH
SystemLabel.DRHO
SystemLabel.VH
SystemLabel.VT

MACROAVE

Prepare the input file macroave.in

```
$ ~/siesta/Util/Macroave/Src/macroave.x
```

You do not need to rerun SIESTA to run MACROAVE as many times as you want

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

The same code with the same input runs with information provided by

Siesta **or** **Abinit**

(indeed it should be quite straight forward to generalize to any other code)

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

Name of the magnitude that will be nanosmoothed

Potential:	**SystemLabel.VH**
Charge:	**SystemLabel.RHO**
TotalCharge:	**SystemLabel.TOCH**

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

SystemLabel

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

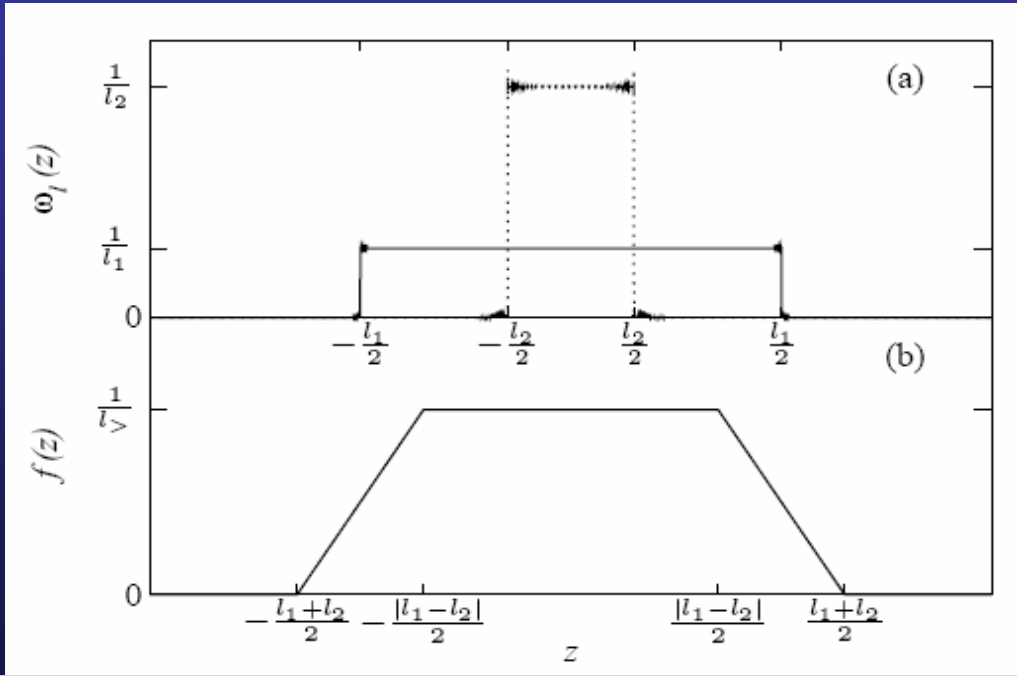
Number of square filter functions used for nanosmoothing

1	Surfaces
2	Interfaces and superlattices

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

Length of the different square filter functions (in bohrs)



Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

Total number of electrons

(used only to renormalize if we nanosmooth the electronic charge)

Input of MACROAVE: macroave.in

```
Siesta              # Which code have you used to get the input data?
Potential           # Quantity that will be nanosmoothed
Interface           # Name of the file where the input data is stored
2                   # Number of convolutions required to calculate the macro. ave.
7.47622255          # First length for the filter function in macroscopic average
7.56114385          # Second length for the filter function in macroscopic average
500                 # Total number of electrons
spline              # Type of interpolation
```

Type of interpolation from the SIESTA mesh to a FFT mesh

Spline or **Linear**

Output of MACROAVE

Planar average

$$\overline{\rho}(z) = \frac{1}{S}\int_S dxdy\ \rho(\vec{r})$$

SystemLabel.PAV

Nanosmoothed

$$\overline{\overline{\rho}}(z) = \int dz'\, f(z - z')\overline{\rho}(z')$$

SystemLabel.MAV

Format

z	average
0.000000000000	0.000000000000
0.000095367432	0.000000000000
0.000190734863	0.000000000000
.	.
.	.
.	.

Units

Coordinates: bohr

Potential: eV

Charge density: electrons/bohr^3

To learn more on nanosmoothing and how to compute work functions and band offsets with SIESTA

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 213203 (34pp) doi:10.1088/0953-8984/19/21/213203

TOPICAL REVIEW

Nanoscale smoothing and the analysis of interfacial charge and dipolar densities

Javier Junquera[1,2], Morrel H Cohen[2,3] and Karin M Rabe[2]

PHYSICAL REVIEW B **67**, 155327 (2003)

First-principles calculation of the band offset at $BaO/BaTiO_3$ and $SrO/SrTiO_3$ interfaces

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