LDA+U

How to run a simulation within LDA+U framework in SIESTA

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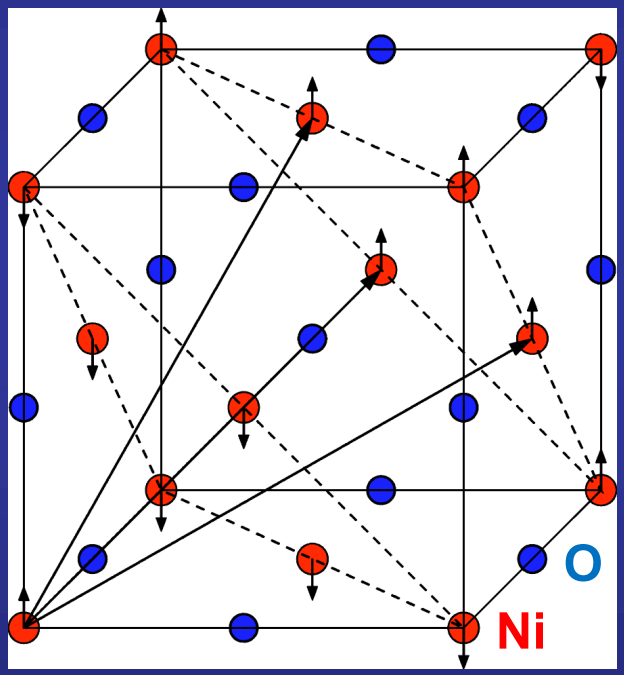
Transition metal monoxides are prototypes of highly correlated materials

Paradigmatic example: NiO

Above the Néel temperature of $T_N = 524$ K is a paramagnetic insulator with the rocksalt structure

Below T_N it is a type-II antiferromagnetic insulator



NiO crystallizes in the rocksalt structure with rhombohedral symmetry induced by the type-II AFM order

Ground state:
Type-II AntiFerroMagnetic:

ferromagnetic alignment of the Ni atoms within the (111) planes and the antiferromagnetic alignment of those planes

M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

Transition metal monoxides are prototypes of highly correlated materials

Paradigmatic example: NiO

Above the Néel temperature of $T_N = 524$ K is a paramagnetic insulator with the rocksalt structure

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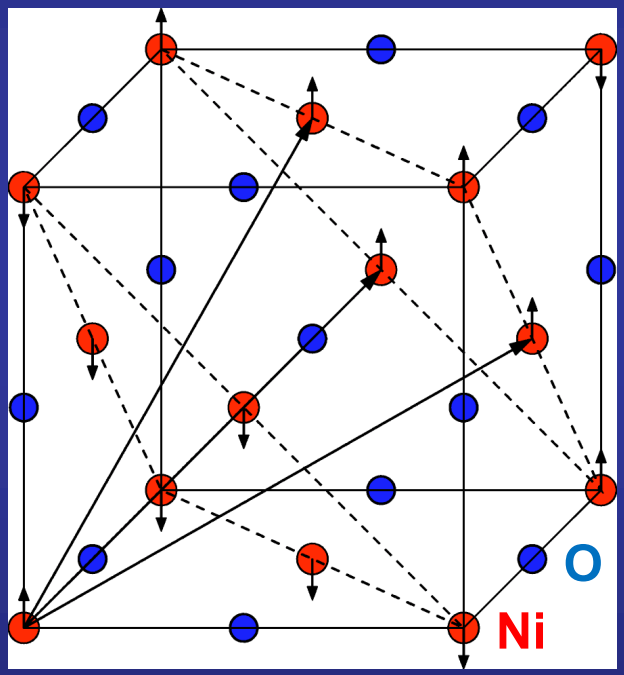


NiO crystallizes in the rocksalt structure with rhombohedral symmetry induced by the type-II AFM order

```
%block Chemical_Species_Label
  1   28    Ni
  2    8     O
%endblock Chemical_Species_Label

#
# Lattice, coordinates, k-sampling
#

LatticeConstant     4.17 Ang

%block LatticeVectors
 1.00      0.50      0.50
 0.50      1.00      0.50
 0.50      0.50      1.00
%endblock LatticeVectors

AtomicCoordinatesFormat Fractional      # Format for coordinates
%block AtomicCoordinatesAndAtomicSpecies
 0.000   0.000   0.000  1   #Atom 1: Ni (Atomic species number 1)
 0.500   0.500   0.500  1   #Atom 2: Ni (Atomic species number 1)
 0.250   0.250   0.250  2   #Atom 3: O  (Atomic species number 2)
 0.750   0.750   0.750  2   #Atom 4: O  (Atomic species number 2)
%endblock AtomicCoordinatesAndAtomicSpecies

SpinPolarized           .true.      # Spin polarized calculation

# For an AFM-Type II structure, choose the following
%block DM.InitSpin       # Describe the initial magnetic order (on Ni only)
 1   +
 2   -
%endblock DM.InitSpin
```

Calculations carried out in the undistorted unit cell at the experimental lattice constant

M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

Band structure of NiO within the generalized grandient approximation

We plot the band structure using the Utility program gnubands, and following the recipe given in the tutorial

Band structure of an ionic solid: the case of MgO

Introduce the path in k-space in the SIESTA input file

```
BandLinesScale      ReciprocalLatticeVectors
%block BandLines
      1  0.000      0.000      0.000     \Gamma
     40  0.500      0.000      0.000     L
     20  0.81250    0.34375    0.34375   K
     40  0.500      0.500      0.500     T
     40  0.000      0.000      0.000     \Gamma
     40  0.500      0.500      0.000     X
%endblock BandLines
```

Run SIESTA, run gnubands and plot the results

```
$ <your_path_to_SIESTA_executable_file>/siesta < NiO_AF2.noU.fdf > NiO_AF2.noU.out
```

Edit the file where the bands along the high-symmetry lines are dumped and identify the top of the valence band eigenvalue. In this example, it amounts to -5.7677 eV

Band structure of NiO within the generalized grandient approximation

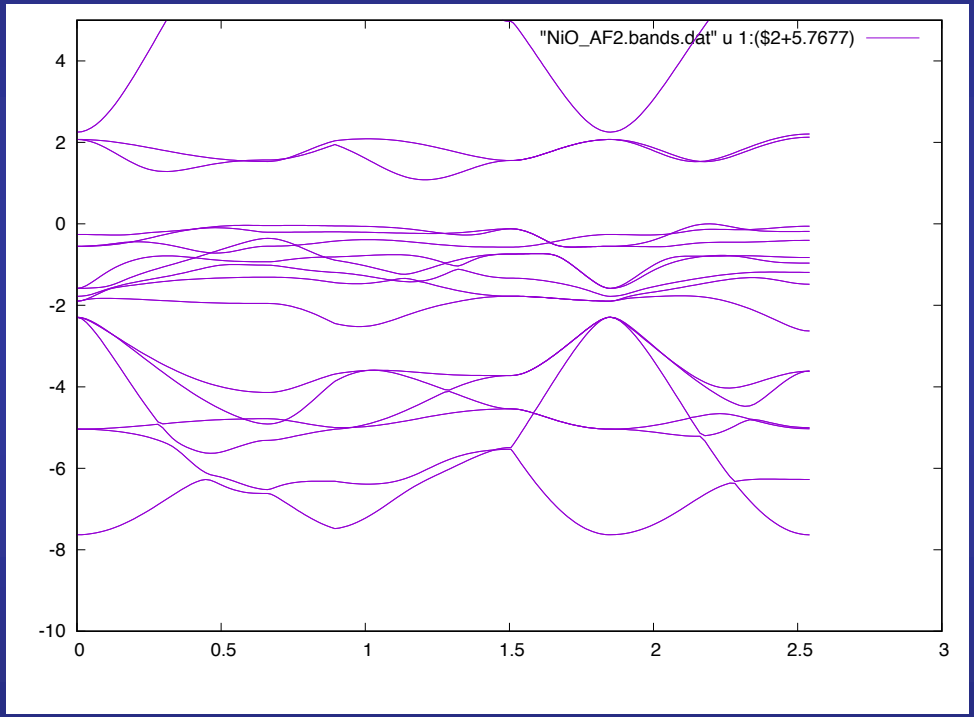
Run gnubands and plot the results

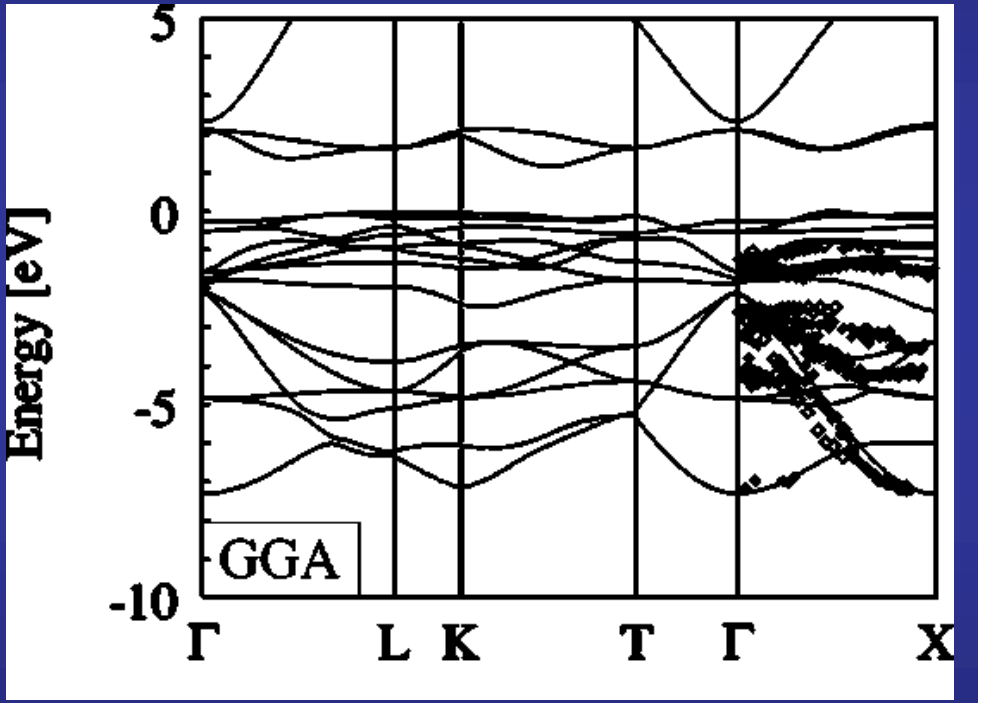
```
$ <your_path_to_SIESTA_dir>/Util/Bands/gnubands < NiO_AF2_noU.bands > NiO_AF2_noU.bands.dat
$ gnuplot
gnuplot> plot "NiO_AF2_noU.bands.dat" using 1:($2+5.7677) with lines
gnuplot> set yrange [-10:5]
gnuplot> replot
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "NiO_AF2_noU.bands.ps"
gnuplot> replot
```

We shift rigidly the bands to set the zero of energy with the top of the valence band

Band structure of NiO within the generalized grandient approximation

Run gnubands and plot the results





This work

M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

GGA gap is too small for NiO

Projected Density of States of NiO within the generalized grandient approximation

We plot the PDOS using the Utility program fmpdos, and following the recipe given in the tutorial

Density of States and Projected Density of States: the case of $SrTiO_3$

Take a look at the fdf input file and study the meaning of the following blocks

```
%block PDOS.kgrid_Monkhorst_Pack
30  0  0  0.5
 0 30  0  0.5
 0  0 30  0.5
%endblock PDOS.kgrid_Monkhorst_Pack
%block ProjectedDensityOfStates
 -25.0  10.0  0.150  3000   eV
%endblock ProjectedDensityOfStates
```

Projected Density of States of NiO within the generalized grandient approximation

```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_noU.PDOS
  Output file name :
Ni_AF2_noU.4s.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
1
  Extract data for n= ... (0 for all n ):
4
  Extract data for l= ... (-1 for all l ):
0
  Extract data for m= ... (9 for all m ):
9
```

Project on the 4*s* orbitals of the Ni atom

```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_noU.PDOS
  Output file name :
Ni_AF2_noU.3d.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
1
  Extract data for n= ... (0 for all n ):
3
  Extract data for l= ... (-1 for all l ):
2
  Extract data for m= ... (9 for all m ):
9
```

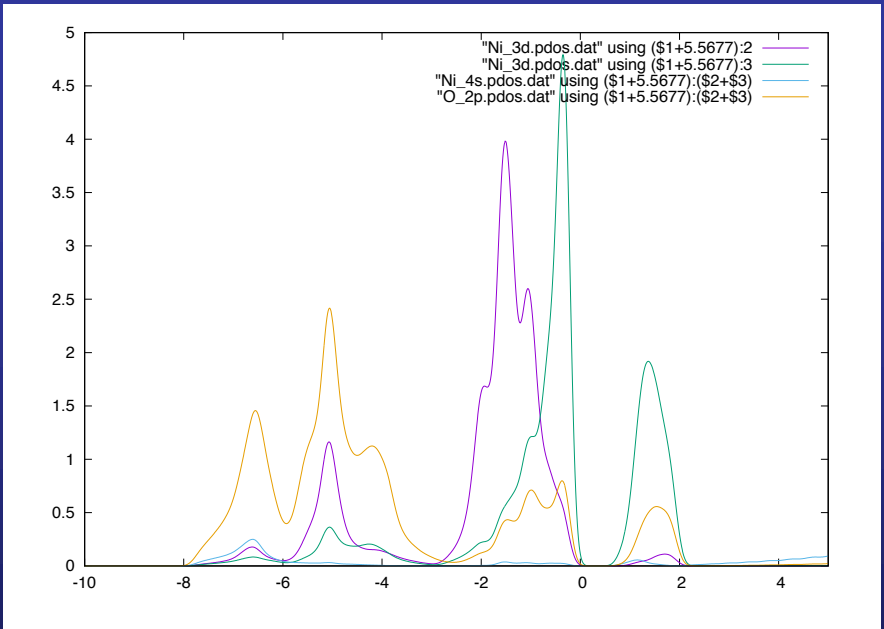
Project on the 3*d* orbitals of the Ni atom

```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_noU.PDOS
  Output file name :
O_AF2_noU.2p.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
3
  Extract data for n= ... (0 for all n ):
2
  Extract data for l= ... (-1 for all l ):
1
  Extract data for m= ... (9 for all m ):
9
```

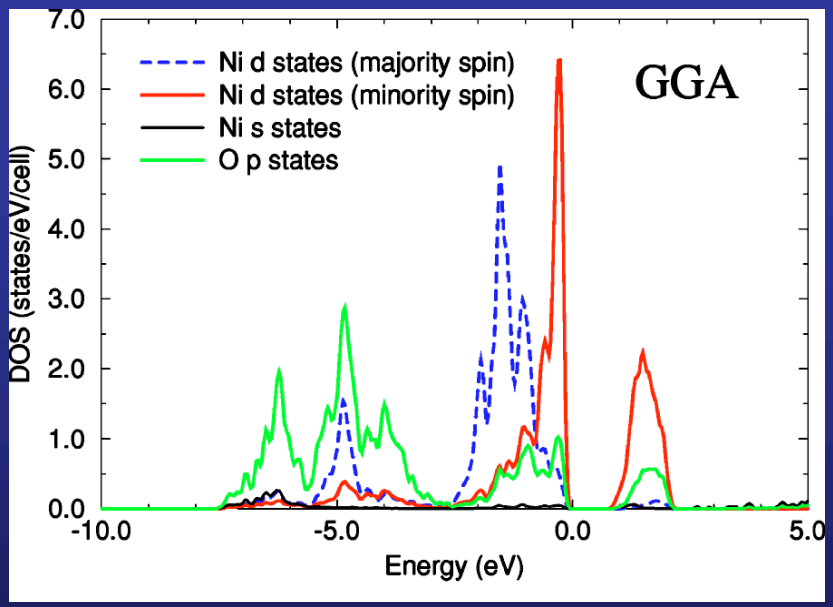
Project on the 2*p* orbitals of the O atom

Projected Density of States of NiO within the generalized grandient approximation

```
$ gnuplot
gnuplot> plot "Ni_AF2_noU.3d.pdos.dat" using ($1+5.5677):2 with lines,
"Ni_AF2_noU.3d.pdos.dat" using ($1+5.5677):3 with lines,
"Ni_AF2_noU.4s.pdos.dat" using ($1+5.5677):($2+$3) with lines,
"O_AF2_noU.2p.pdos.dat" using ($1+5.5677):($2+$3) with lines
gnuplot> set xrange [-10:5]
gnuplot> replot
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "NiO_AF2_noU.PDOS.ps"
gnuplot> replot
```



This work



M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

How to introduce the U

LDA+U method

LDA (or GGA) is supplemented with a Hubbard-like term in order to have a better description of the effect of electron-electron interactions in a localized atomic shell of a particular atom in the solid, i.e. 3d shell of Ni in NiO

In particular this reduces the problem of Self-Interaction

$$E^{\mathrm{LDA+U}} = E^{\mathrm{LDA}} + U n_\uparrow n_\downarrow - \frac{U}{2} N(N-1)$$

with

$$n_\sigma = \langle \hat{n}_\sigma \rangle$$

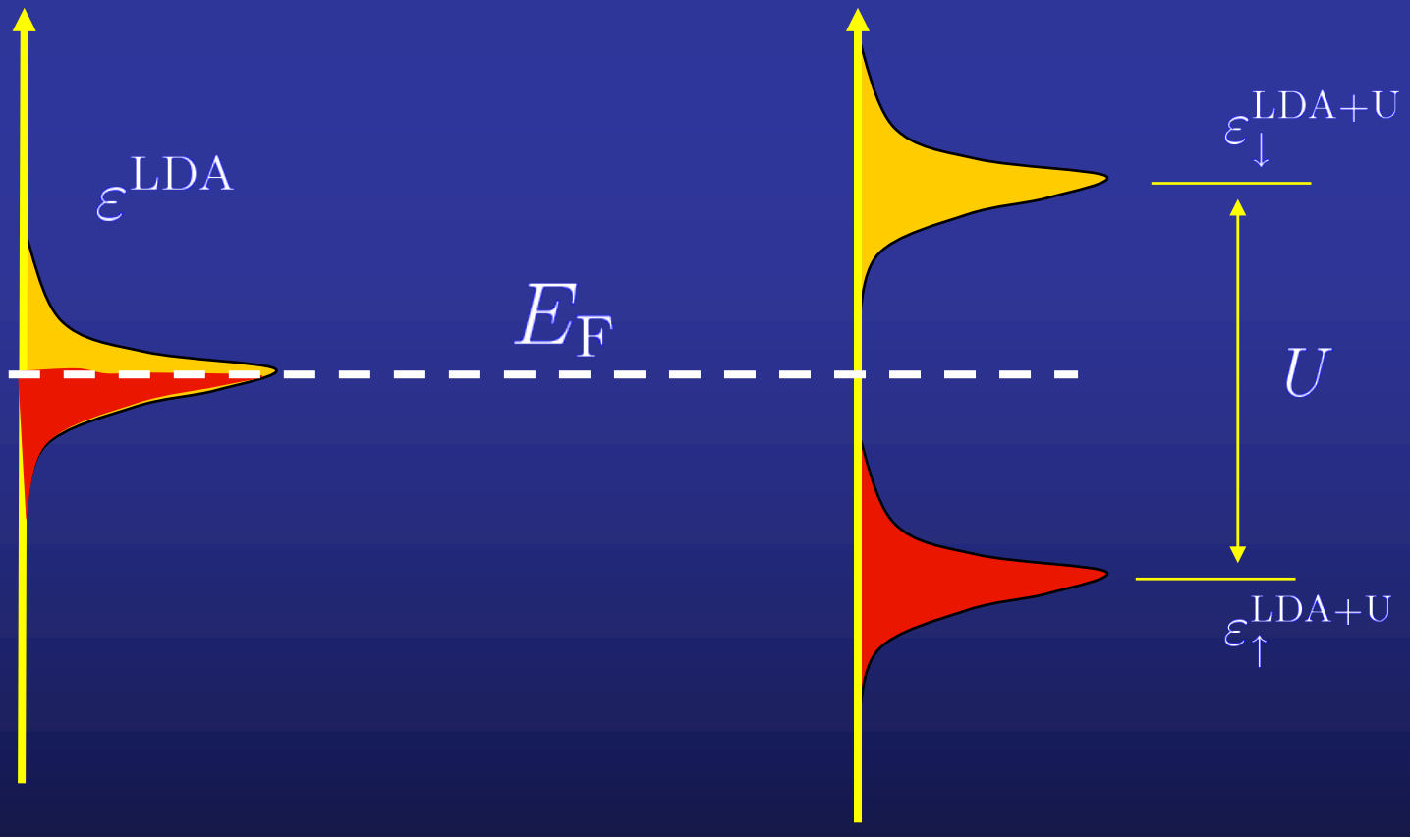
$$N = n_\uparrow + n_\downarrow$$

Double counting term (cancels the electron-electron interaction in the localized shell in LDA)

LDA+U method

$$\hat{H}_\sigma^{\mathrm{LDA+U}} = \frac{\delta E^{\mathrm{LDA+U}}}{\delta \langle \psi_\sigma |} = \hat{H}_\sigma^{\mathrm{LDA}} + U \left(\frac{1}{2} - n_\sigma \right) \hat{n}_\sigma$$

$$\varepsilon_\sigma^{\mathrm{LDA+U}} = \frac{\delta E^{\mathrm{LDA+U}}}{\delta n_\sigma} = \varepsilon_\sigma^{\mathrm{LDA}} + U \left(\frac{1}{2} - n_\sigma \right)$$



Rotationally invariant formulation

$$n_{mm'} = \sum_{n \in \mathrm{occ}} \langle \Psi_n | \phi_m \rangle \langle \phi_{m'} | \Psi_n \rangle$$

$$E^{\mathrm{LDA+U}} = E^{\mathrm{LDA}} + \frac{U^{\mathrm{eff}}}{2} \left[\underleftrightarrow{n} - \underleftrightarrow{n}\,\underleftrightarrow{n} \right]$$

Dudarev *et al.*, Phys. Rev. B 57, 1505 (1998)

Populations are calculated using localized projectors

$$n_i = \sum_{n \in \mathrm{occ}} \langle \Psi_n | \phi_i \rangle \langle \phi_i | \Psi_n \rangle$$

Two different ways of define the projectors, selected with the keyword LDAU.ProjectorGenerationMethod

Method 1: Generated in the same way as a simple-ζ orbital, with a larger Energy Shift

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

Method 1: Generated in the same way as a simple-ζ orbital, with a larger Energy Shift

```
LDAU.ProjectorGenerationMethod 1
```

The Schrödinger equation for the isolated atom might be solved with a confinement potential, in the same way as it is done for the basis atomic orbitals

```
%block LDAU.Proj       # Define LDA+U projectors
 Mn    2               # Label, l_shells
  n=3 2  E 50.0 2.5    # n (opt if not using semicore levels),l,Softconf(opt)
       5.00  0.35      # U(eV), J(eV) for this shell
       2.30            # rc (Bohr)
       0.95            # scaleFactor (opt)
       0               #    l
       1.00  0.05      # U(eV), J(eV) for this shell
       0.00            # rc(Bohr) (if 0, automatic r_c from LDAU.EnergyShift)
%endblock LDAU.Proj
```

We are going to generate two projectors for a Mn atom

The first one, for the 3d shell
(we can specify both n and l quantum numbers)

The second one, for the 4s shell
(here we only specify the l quantum number)
(might be quite unphysical… only shown here as an example to tell how the projectors are introduced)

Method 1: Generated in the same way as a simple-ζ orbital, with a larger Energy Shift

```
LDAU.ProjectorGenerationMethod 1
```

```
%block LDAU.Proj       # Define LDA+U projectors
 Mn    2               # Label, l_shells
  n=3 2  E 50.0 2.5    # n (opt if not using semicore levels),l,Softconf(opt)
       5.00  0.35      # U(eV), J(eV) for this shell
       2.30            # rc (Bohr)
       0.95            # scaleFactor (opt)
       0               #    l
       1.00  0.05      # U(eV), J(eV) for this shell
       0.00            # rc(Bohr) (if 0, automatic r_c from LDAU.EnergyShift)
%endblock LDAU.Proj
```

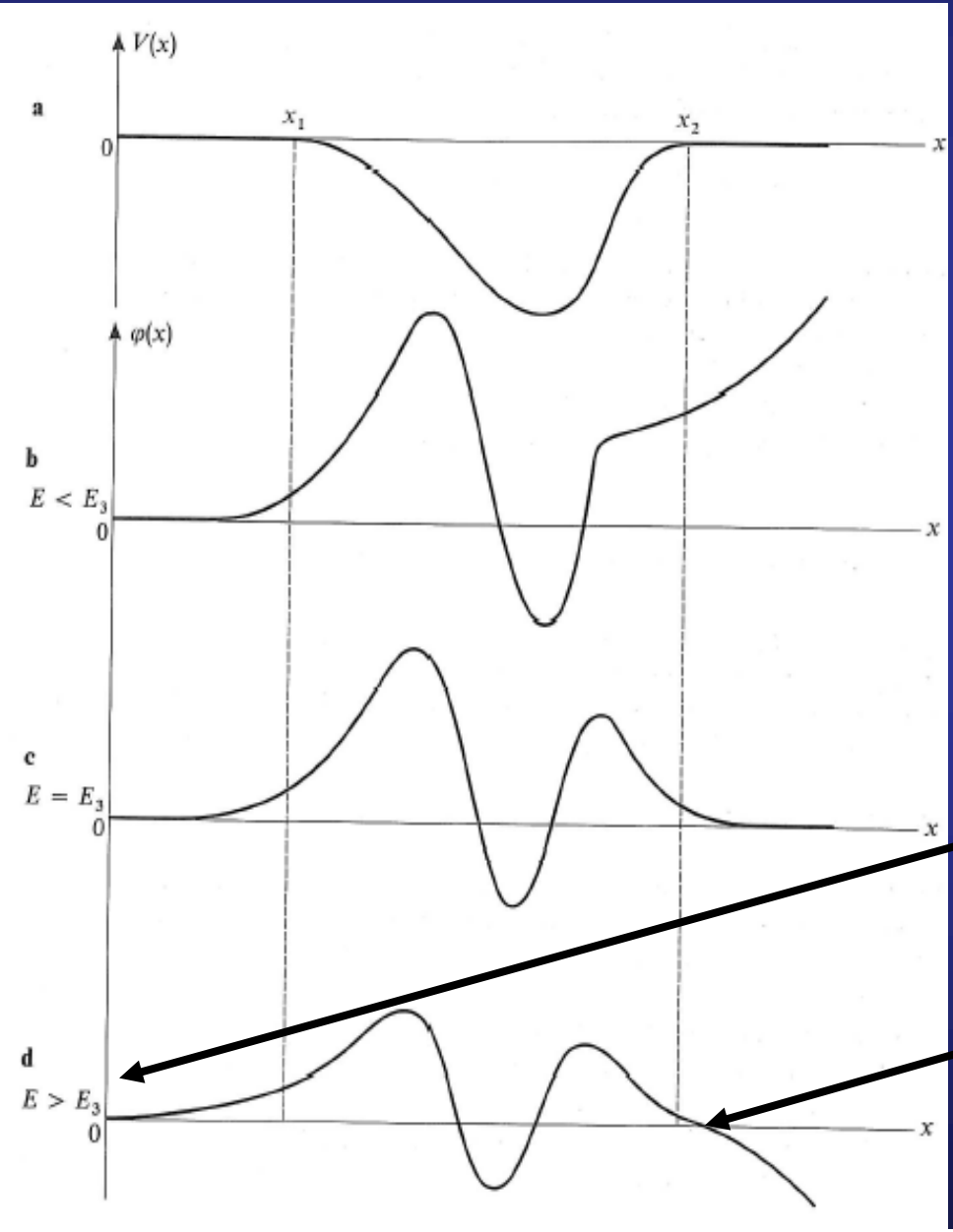
The **cutoff radius of the LDA+U projector**, r_c, can be explicitly introduced in the block LDAU.Proj.

If it appears as zero in the block, the value introduced in the **LDAU.EnergyShift** label is used

(Default value 0.05 Ry)

LDAU.EnergyShift is the same as the parameter PAO.EnergyShift: the energy increase used to define the localization radius of the LDA+U projector r_c

How to control the range of the orbitals in a balanced way: the energy shift



Particle in a confinement potential:

Imposing a finite $\int_{-\infty}^{+\infty} |\phi(x)|^2 dx$

Continuous function and first derivative

$\Downarrow$

E is quantized (not all values allowed)

Increasing $E \Rightarrow \phi_\mu$ has a node and tends to -∞ when $x \rightarrow$ + ∞

Complement M III "Quantum Mechanics",

C. Cohen-Tannoudji *et al.*

How to control de range of the orbitals in a balanced way: the energy shift

$$\left(-\frac{1}{2r}\frac{d^2}{dr^2}r+\frac{l(l+1)}{2r^2}+V_l(r)\right)R_l(r)=(\varepsilon_l+\delta\varepsilon_l)\,R_l(r)$$

Energy increase ≡ Energy shift

LDAU.EnergyShift (energy)

Cutoff radius, r_c, = position where each orbital has the node

A **single parameter for all** cutoff radii

The larger the Energy shift, the shorter the r_c's

Typical values for generating basis sets: 100-200 meV

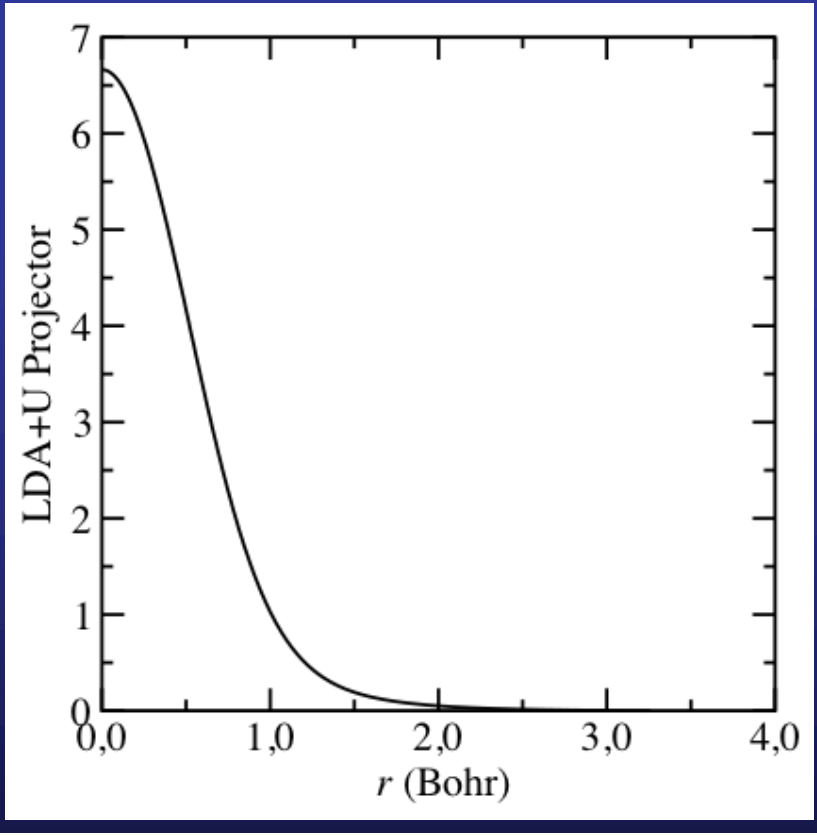
LDA+U projectors should be rather localized, therefore larger EnergyShifts are expected

E. Artacho et al. Phys. Stat. Solidi (b) 215, 809 (1999)

Method 1: Generated in the same way as a simple-ζ orbital, with a larger Energy Shift

```
LDAU.ProjectorGenerationMethod 1
```

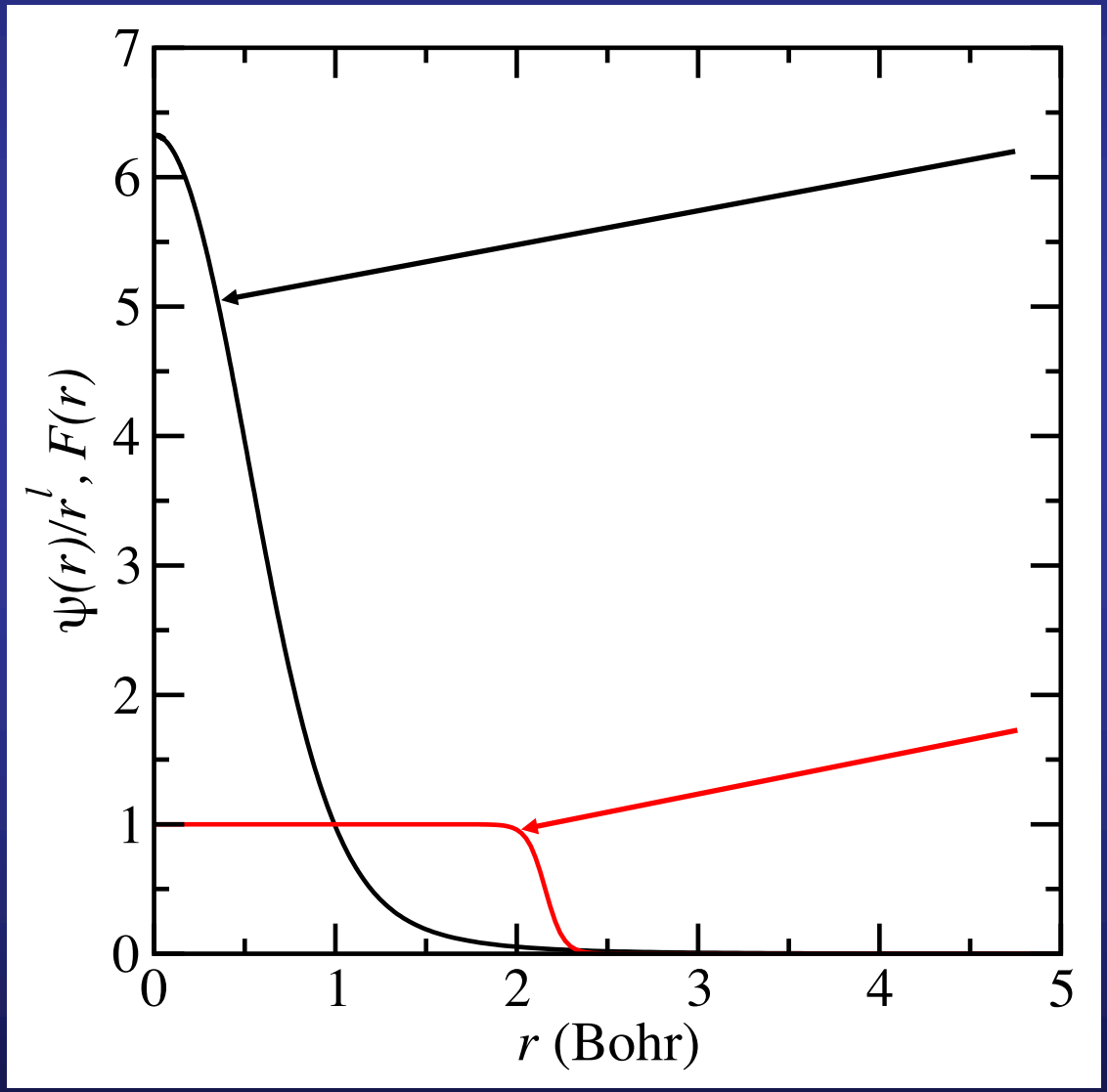
If the label WritelonPlotFiles is set to .true.
Then the radial part pf the projectors is written in the file
LDA+U.LX.Y.AtomicSymbol
X = Angular momentum
Y= number of projector for this angular momentum



What is represented is the radial part divided by r^l

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

```
LDAU.ProjectorGenerationMethod 2
```



Solve the Schrödinger equation for the isolated atom with a large cutoff

Multiply the long wave function by a Fermi function

$$F(r_c, \omega) = \frac{1}{1 + \exp(\frac{r - r_c}{\omega})}$$

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

`LDAU.ProjectorGenerationMethod 2`

The Schrödinger equation for the isolated atom might be solved with a confinement potential, in the same way as it is done for the basis atomic orbitals (although, since we need a long wave function, it is recommended not to confine them)

```
%block LDAU.Proj      # Define LDAU projectors
 Mn    2              # Label, l_shells
  n=3 2  E 50.0 2.5   # n (opt if not using semicore levels),l,Softconf(opt)
       5.00  0.35     # U(eV), J(eV) for this shell
       2.30  0.15     # rc (Bohr), \omega(Bohr) (Fermi cutoff function)
       0.95           # scaleFactor (opt)
       0              #    l
       1.00  0.05     # U(eV), J(eV) for this shell
       0.00  0.00     # rc(Bohr), \omega(Bohr) (if 0 r_c from LDAU.CutoffNorm
%endblock LDAU.Proj   #                          and \omega from default value)
```

We are going to generate two projectors for a Mn atom

The first one, for the 3d shell
(we can specify both n and l quantum numbers)

The second one, for the 4s shell
(here we only specify the l quantum number)
(might be quite unphysical… only shown here as an example to tell how the projectors are introduced)

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

`LDAU.ProjectorGenerationMethod 2`

How to determine the parameters of the Fermi function

$$F(r_c, \omega) = \frac{1}{1 + \exp(\frac{r - r_c}{\omega})}$$

`LDAU.ProjectorGenerationMethod 2`

```
%block LDAU.Proj      # Define LDAU projectors
 Mn    2              # Label, l_shells
  n=3 2  E 50.0 2.5   # n (opt if not using semicore levels),l,Softconf(opt)
      5.00  0.35      # U(eV), J(eV) for this shell
      2.30  0.15      # rc (Bohr), \omega(Bohr) (Fermi cutoff function)
      0.95            # scaleFactor (opt)
      0               #    l
      1.00  0.05      # U(eV), J(eV) for this shell
      0.00  0.00      # rc(Bohr), \omega(Bohr) (if 0 r_c from LDAU.CutoffNorm
%endblock LDAU.Proj   #                          and \omega from default value)
```

The cutoff radius of the Fermi function, r_c, equivalent to the Fermi energy, can be explicitly introduced in the block LDAU.Proj.

If it appears as zero in the block, the value introduced in the LDAU.CutoffNorm label is used

(Default value 0.90)

LDAU.CutoffNorm is the norm of the original pseudoatomic orbital contained in a sphere of radius equal to r_c

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

`LDAU.ProjectorGenerationMethod 2`

How to determine the parameters of the Fermi function

$$F(r_c, \omega) = \frac{1}{1 + \exp\left(\frac{r - r_c}{\omega}\right)}$$

`LDAU.ProjectorGenerationMethod 2`

```
%block LDAU.Proj      # Define LDAU projectors
 Mn    2              # Label, l_shells
  n=3 2  E 50.0 2.5   # n (opt if not using semicore levels),l,Softconf(opt)
      5.00  0.35      # U(eV), J(eV) for this shell
      2.30  0.15      # rc (Bohr), \omega(Bohr) (Fermi cutoff function)
      0.95            # scaleFactor (opt)
      0               #    l
      1.00  0.05      # U(eV), J(eV) for this shell
      0.00  0.00      # rc(Bohr), \omega(Bohr) (if 0 r_c from LDAU.CutoffNorm
%endblock LDAU.Proj   #                          and \omega from default value)
```

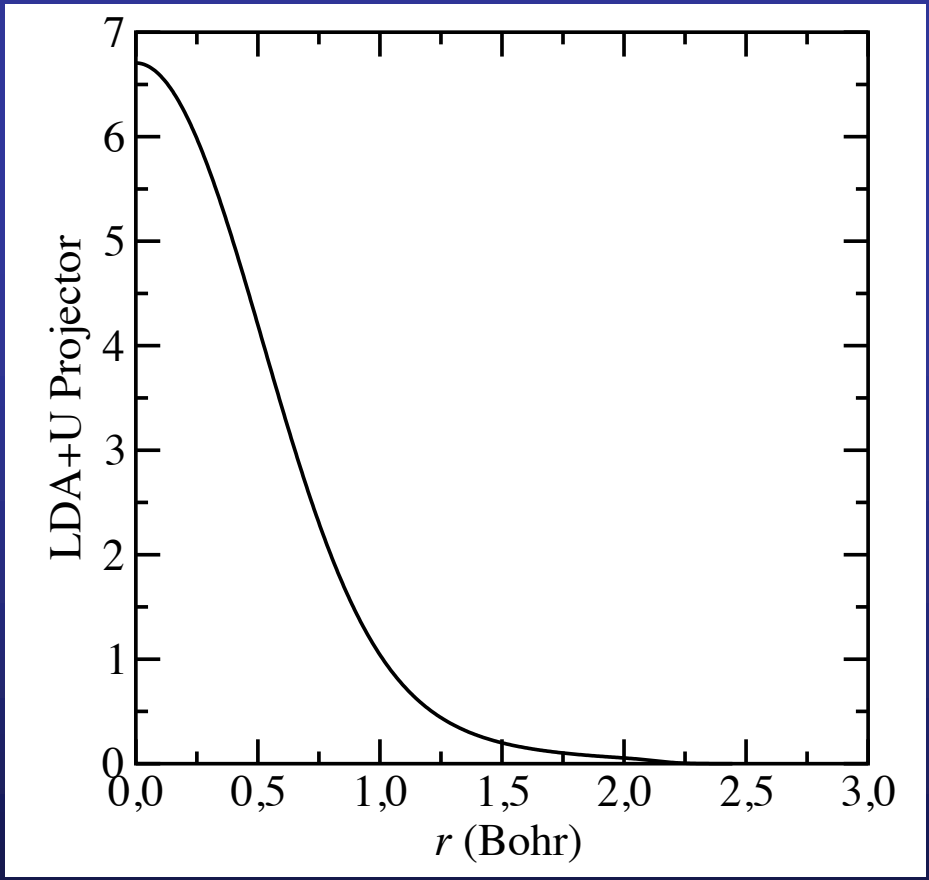
The width of the Fermi function, ω, is controlled by the parameters included in the block LDAU.Proj.

If it appears as zero in the block, a default value of 0.05 will be used

Method 2: Cut the exact solution of the pseudoatomic problem with a Fermi function

`LDAU.ProjectorGenerationMethod 2`

If the label WritelonPlotFiles is set to .true.
Then the radial part pf the projectors is written in the file
LDA+U.LX.Y.AtomicSymbol
X = Angular momentum
Y= number of projector for this angular momentum



What is represented is the radial part divided by r^l

Populations are calculated using localized projectors

In the NiO example, we have used the
LDAU.ProjectorGenerationMethod 2

```
LDAU.ProjectorGenerationMethod   2
LDAU.CutoffNorm                  0.90

%block LDAU.proj
Ni 1          # number of shells of projectors
n=3 2         # n, l
4.600 0.000 # U(eV), J(eV)
0.000 0.000 # rc, \omega (default values)
%endblock LDAU.proj
```

The equivalent to the Fermi energy of the Fermi function is chosen using the LDAU.CutoffNorm parameter
And for the width we rely on the default value

Main keywords related with the U parameter

```
LDAU.ProjectorGenerationMethod   2
LDAU.CutoffNorm                  0.90

%block LDAU.proj
Ni 1          # number of shells of projectors
n=3 2         # n, l
4.600 0.000   # U(eV), J(eV)
0.000 0.000   # rc, \omega (default values)
%endblock LDAU.proj
```

Main keywords related with the LDA+U self-consistency

```
LDAU.FirstIteration                .false.
LDAU.ThresholdTol                  1.0d-3
LDAU.PopTol                        4.0d-4
```

LDAU.FirstIteration

If true, local populations are calculated and Hubbard-like term is switch on in the first iteration. Useful if restarting a calculation reading a converged or an almost converged density matrix from file.

LDAU.ThresholdTol

Local populations only calculated and/or updated if the change in the density matrix elements (dDmax) is lower than LDAU.ThresholdTol.

LDAU.PopTol

Convergence criterium for the LDA+U local populations. In the current implementation the Hubbard-like term of the Hamiltonian is only updated (except for the last iteration) if the variations of the local populations are larger than this value.

Band structure of NiO within the generalized grandient approximation + U

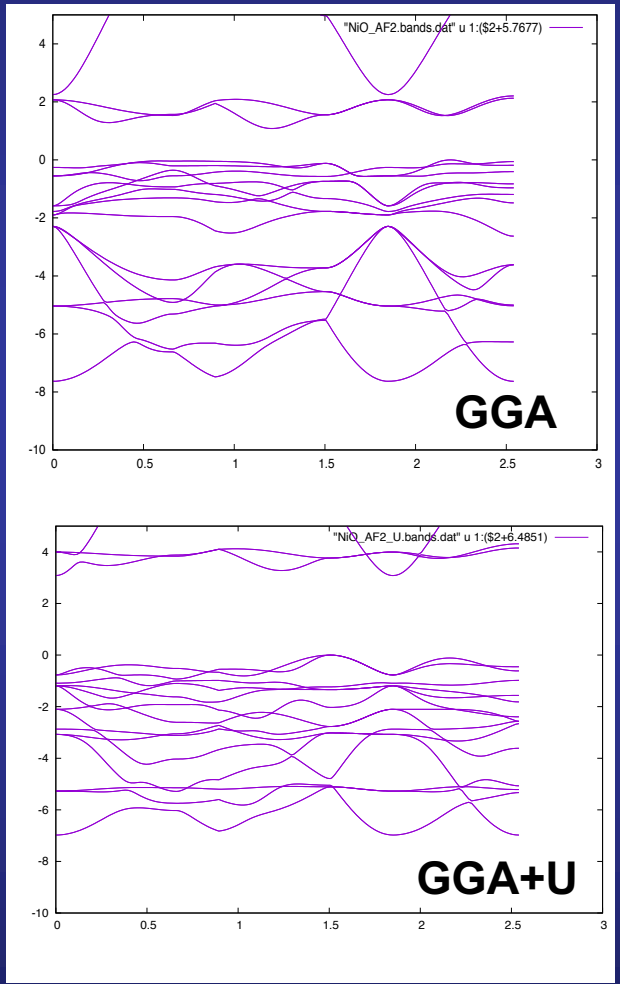
Run SIESTA, and then run gnubands and plot the results

```
$ <your_path_to_SIESTA_executable>/siesta < NiO_AF2.U.fdf > NiO_AF2.U.out

$ <your_path_to_SIESTA_dir>/Util/Bands/gnubands < NiO_AF2.U.bands > NiO_AF2.U.bands.dat

$ gnuplot
gnuplot> plot "NiO_AF2_U.bands.dat" u 1:($2+6.4851) with lines
gnuplot> set yrange [-10:5]
gnuplot> replot
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "NiO_AF2_U.bands.ps"
gnuplot> replot
```

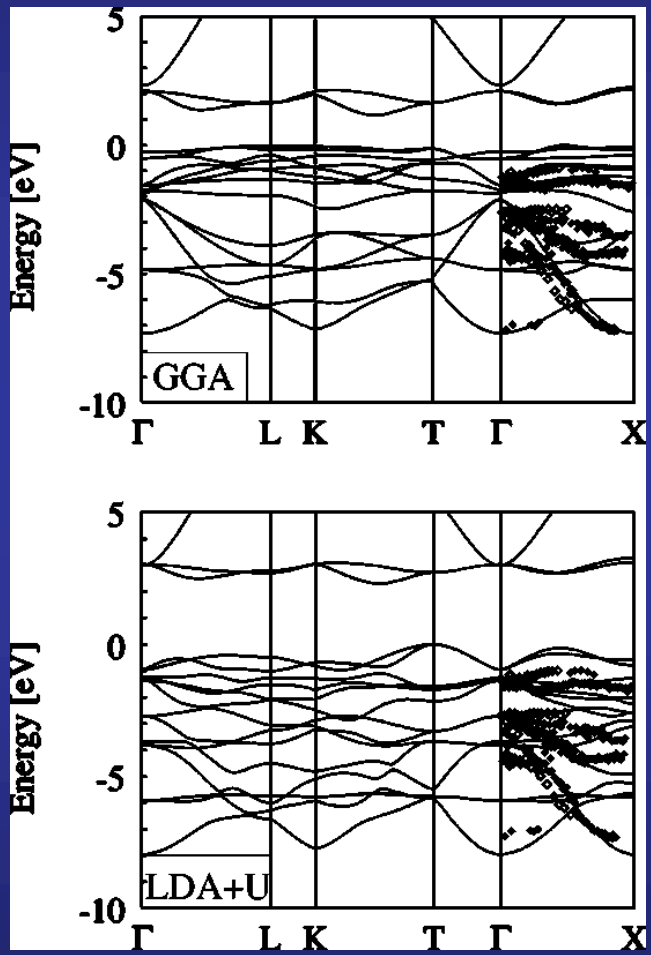
We shift rigidly the bands to set the zero of energy with the top of the valence band

Band structure of NiO within the generalized grandient approximation + U

Run gnubands and plot the results



This work



M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

Projected Density of States of NiO within the generalized grandient approximation + U

```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_U.PDOS
  Output file name :
Ni_4s.AF2.U.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
1
  Extract data for n= ... (0 for all n ):
4
  Extract data for l= ... (-1 for all l ):
0
  Extract data for m= ... (9 for all m ):
9
```

Project on the 4*s* orbitals of the Ni atom

```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_U.PDOS
  Output file name :
Ni_3d.AF2.U.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
1
  Extract data for n= ... (0 for all n ):
3
  Extract data for l= ... (-1 for all l ):
2
  Extract data for m= ... (9 for all m ):
9
```

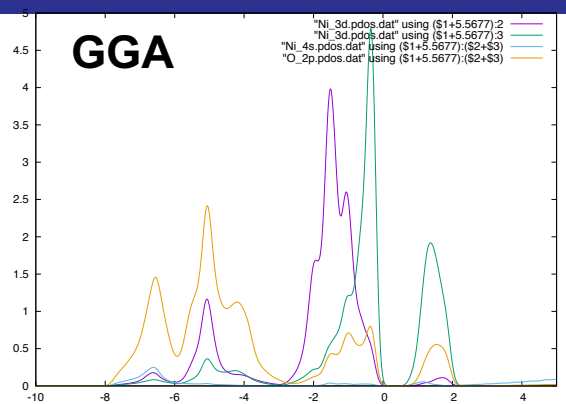
Project on the 3*d* orbitals of the Ni atom

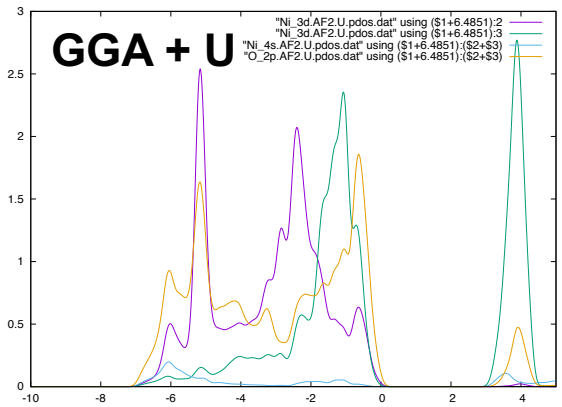
```
$ <your_path_to_SIESTA_dir>/Util/Contrib/APostnikov/fmpdos
  Input file name (PDOS):
NiO_AF2_U.PDOS
  Output file name :
O_2p.AF2.U.pdos.dat
  Extract data for atom index (enter atom NUMBER, or 0 to select all),
  or for all atoms of given species (enter its chemical LABEL):
3
  Extract data for n= ... (0 for all n ):
2
  Extract data for l= ... (-1 for all l ):
1
  Extract data for m= ... (9 for all m ):
9
```

Project on the 2*p* orbitals of the O atom

Projected Density of States of NiO within the generalized grandient approximation + U

```
$ gnuplot
gnuplot> plot "Ni_3d.AF2.U.pdos.dat" using ($1+6.4851):2 with lines,
"Ni_3d.AF2.U.pdos.dat" using ($1+6.4851):3 with lines,
"Ni_4s.AF2.U.pdos.dat" using ($1+6.4851):($2+$3) with lines,
"O_2p.AF2.U.pdos.dat" using ($1+6.4851):($2+$3) with lines
gnuplot> set xrange [-10:5]
gnuplot> replot
gnuplot> set terminal postscript color
Terminal type set to 'postscript'
Options are 'landscape enhanced defaultplex \
   leveldefault color colortext \
   dashlength 1.0 linewidth 1.0 butt noclip \
   nobackground \
   palfuncparam 2000,0.003 \
   "Helvetica" 14  fontscale 1.0 '
gnuplot> set output "NiO_AF2_U.pdos.ps"
gnuplot> replot
```





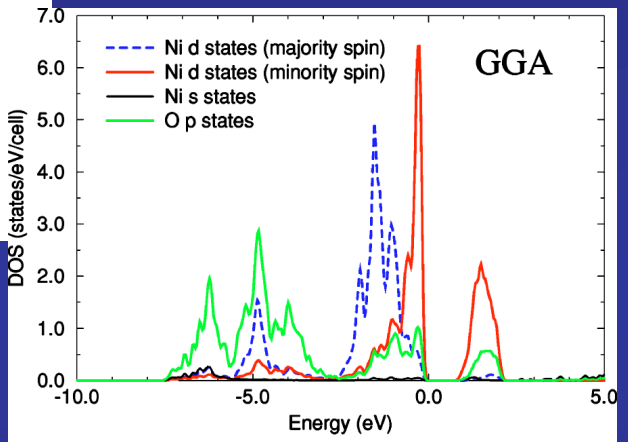
This work

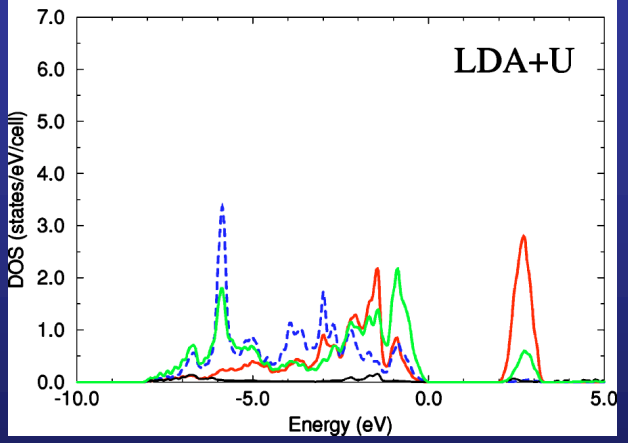
GGA+U qualitatively modifies the nature of the states at the top of the valence band, and hence the nature of the band gap

GGA: Ni d states

GGA+U: O p states

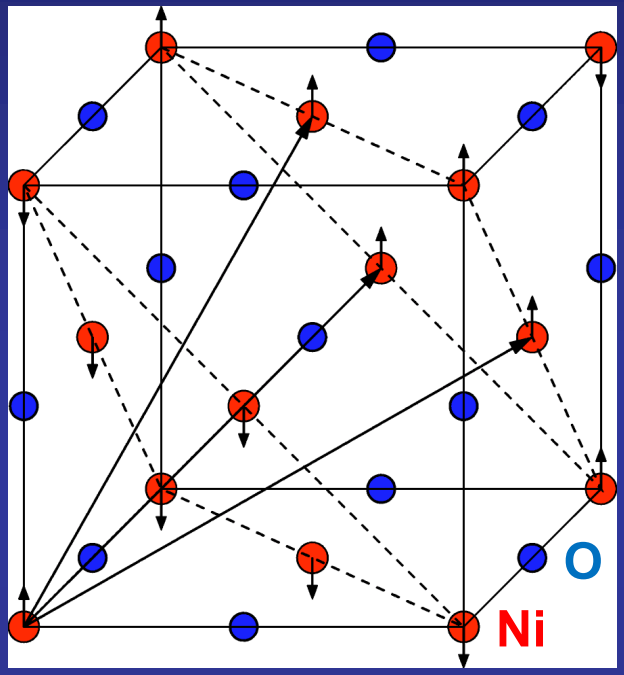
The bottom of the conduction band is of Ni d character, so the predicted band-gap is of charge-transfer type within GGA+U, in good agreement with experiment.





M. Cococcioni and S. de Gironcoli
Phys. Rev. B 71, 035105 (2005)

Magnetic moment in bulk NiO



NiO crystallizes in the rocksalt structure with rhombohedral symmetry induced by the type-II AFM order

M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005)

WriteMullikenPop 1

```
siesta: Total spin polarization (Qup-Qdown) =     0.000000

mulliken: Atomic and Orbital Populations:

mulliken: Spin UP

Species: Ni
Atom  Qatom  Qorb
                3s       4s       4s       3py      3pz      3px      3dxy     3dyz
                3dz2     3dxz     3dx2-y2  3dxy     3dyz     3dz2     3dxz     3dx2-y2
                4Ppy     4Ppz     4Ppx
   1  9.291   0.997    0.399   -0.180    0.997    0.997    0.997    1.007    1.007
               0.985    1.007    0.985   -0.011   -0.011    0.019   -0.011    0.019

mulliken: Spin DOWN

Species: Ni
Atom  Qatom  Qorb
                3s       4s       4s       3py      3pz      3px      3dxy     3dyz
                3dz2     3dxz     3dx2-y2  3dxy     3dyz     3dz2     3dxz     3dx2-y2
                4Ppy     4Ppz     4Ppx
   1  7.619   0.998    0.414   -0.195    1.004    1.004    1.004    1.031    1.031
               0.182    1.031    0.182   -0.038   -0.038   -0.018   -0.038   -0.018
```

GGA +U $\mu = 1.672\ \mu_B$

Well within the experimental ranges of values (from 1.64 to 1.9)

GGA $\mu = 1.393\ \mu_B$

Funding

SPANISH INITIATIVE FOR ELECTRONIC SIMULATIONS WITH THOUSANDS OF ATOMS: CÓDIGO ABIERTO CON GARANTÍA Y SOPORTE PROFESIONAL: SIESTA-PRO
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y cofinanciado con Fondos Estructurales de la Unión Europea
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"Promover el desarrollo tecnológico, la innovación y una investigación de calidad"