Calculating the effective U in APW methods. NiO

Georg K. H. Madsen and Pavel Novák
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The following is an example of how to calculate the effective U following the prescription of ref.[1]. The following steps are described

- generating a supercell

- modifying the input files

- Perform the two SCF calculations

- calculating the U from the values in the scf file.

I. GENERATING A SUPERCELL

This can be done in several ways. For the present case we chose a $2 \times 2 \times 2$ F-centered cell. The steps are:

1. set-up the standard F-centered, a=7.927 a.u. NiO.struct file.

2. For this example choose R_{MT} to 2.3 a.u. and 1.65 a.u. for Ni and O respectively. The result shouldn't be too sensitive to these choices.

3. Run supercell and choose a $2 \times 2 \times 2$ F-centered cell.

4. Change the name of the first Ni to Ni1 (to break symmetry). This is your impurity.

5. Run x sgroup and copy NiO.struct_sgroup to NiO.struct. Your struct file should now have the header:

```
NiO
F   LATTICE,NONEQUIV.ATOMS:  5 225 Fm-3m
MODE OF CALC=RELA unit=
 15.854002 15.854002 15.854002 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ni1        NPT=  781  R0=0.00050000 RMT=    2.3000   Z: 28.0
```

II. RUN NORMAL SCF

Run the init as usual. Use just one k-point. For the present choose an Rkmax of 5. The original Anisimov and Gunnarsson[2] force everything but the impurity d states to be non-spinpolarized. This is not really necessary and would make our calculations more complicated. We therefore run the calculation spinpolarized, but start with only the impurity in a spinpolarized states. This also improves convergence. Modify inst so that it looks like:

```
Ni
Ar 3 5
3, 2,2.0  P
3, 2,2.0  P
3,-3,3.0  P
3,-3,1.0  P
4,-1,1.0  N
4,-1,1.0  N
Ni
Ar 3 5
3, 2,2.0  N
3, 2,2.0  N
```

```
3,-3,2.0  N
3,-3,2.0  N
4,-1,1.0  N
4,-1,1.0  N
Ni
Ar 3 5
3, 2,2.0  N
3, 2,2.0  N
3,-3,2.0  N
3,-3,2.0  N
4,-1,1.0  N
4,-1,1.0  N
O
He 3 5
2,-1,1.0  N
2,-1,1.0  N
2, 1,1.0  N
2, 1,1.0  N
2,-2,1.0  N
2,-2,1.0  N
O
He 3 5
2,-1,1.0  N
2,-1,1.0  N
2, 1,1.0  N
2, 1,1.0  N
2,-2,1.0  N
2,-2,1.0  N
****
****

now run

x lstart
x dstart
x dstart -up
x dstart -dn
runsp
save NiO_orig
```

This is actually only to get a good starting density. The results are not needed directly.

III.   MODIFYING THE INPUT FILES

You now need to change in1, in2 and inc to put a constrained number of d-electrons in the core.

A.   Adding d to the core.

Usually Ni^{2+} has 8 d electrons. You now want to perform two calculations. One with 4.5 ↑, 4 ↓ and one with 4.5 ↑, 3 ↓ constrained d-electrons.[1] You thus make 4 .inc files and here the headers are given
The 4.5 ↑, 4 ↓ calculation. First atom

```
NiO.incup_+.50:        NiO.incdn_+.50
 7 1.00                 7 1.00
1,-1,2                 1,-1,2
2,-1,2                 2,-1,2
2, 1,2                 2, 1,2
```

```
2,-2,4                     2,-2,4
3,-1,2                     3,-1,2
3, 2,4                     3, 2,4
3,-3,5                     3,-3,4
```

notice that a shift has been added to improve convergence.
The 4.5 ↑, 3 ↓ calculation. First atom

```
NiO.incup_+.5-1:          NiO.incdn_+.5-1
 7 1.00                    7 1.00
1,-1,2                     1,-1,2
2,-1,2                     2,-1,2
2, 1,2                     2, 1,2
2,-2,4                     2,-2,4
3,-1,2                     3,-1,2
3, 2,4                     3, 2,4
3,-3,5                     3,-3,2
```

B.   Removing impurity d states from valence states

First you want to remove d from impurity basis this is usually done by setting the linearization energy far above the Fermi level. You only need to change one number.[3] The first lines of in1 should now look like

```
WFFIL           (WFPRI, SUPWF)
  5.00        10    4 (R-MT*K-MAX; MAX L IN WF, V-NMT
  0.30    4  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
1    0.30       0.000 CONT 1
1   -4.95       0.005 STOP 1
2   20.30       0.000 CONT 1
0    0.30       0.000 CONT 1
```

Secondly you need to remove the d impurity electrons from the valence. You thus need two in2 files. The original NiO supercell had 176 valence electrons. You have put 8.5 and 7.5 electrons into the core. The header of your in2 files should thus look like

```
NiO.in2_+.50:                  |  NiO.in2_+.5-1:
TOT             (TOT,FOR,QTL,EF |  TOT                (TOT,FOR,QTL,EF
    -9.0      167.5 0.50 0.05   |        -9.0      168.5 0.50 0.05
GAUSS    0.006                  |  GAUSS     0.006
```

The unit-cell neutrality is thus kept. Notice that a GAUSS smearing has been added to improve convergence.

IV.   RUNNING THE SCF

Now you are ready to run the constrained calculations. Run:

```
cp NiO.in2_+.50 NiO.in2
cp NiO.incup_+.50 NiO.incup
cp NiO.incdn_+.50 NiO.incdn
runsp
save NiO_+.50
```

afterwards do the same thing for +.5-1. Usually you can just start from the converged density.

V.   CALCULATING THE U FROM THE VALUES IN THE SCF FILE

To apply Eq. (4)[1] you need four values that can be found in the SCF files.

```
grepline :fer 'NiO_+.50.scf' 1
```

gives $\varepsilon_F((n+1)/2, n/2)$

```
grepline :3dd001 'NiO_+.50.scf' 2 | head -2 | tail -1
grepline ':3d 001' 'NiO_+.50.scf' 2 | head -2 | tail -1
```

Do a weighted sum of these two values $(4*3dd001 + 5*3d001)/9 = \varepsilon_{3d\uparrow}((n+1)/2, n/2)$. And similarly for +.5-1. By applying Eq. (4) you should then get $F_{eff}^0 = 0.438$ Ry= 5.96 eV. In Ref. [1] we argue that you should use this value for U and set J to zero

Have fun

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[1] G. K. H. Madsen and P. Novák, Europhys. Lett. **69**, 777 (2005).
[2] V. I. Anisimov and O. Gunnarsson, Phys. Rev. B **43**, 7570 (1991).
[3] Usually it is bett er to just set the d energy 2-4 Ry above the Fermi level. For the present it shouldn't matter much