Calculation of U for NiO:
1). I have generated the 2 × 2 × 2 F-centered cell, where the parameters are : a=7.927 a.u. and R MT to 2.3 a.u. and 1.65 a.u. for Ni and O respectively.
2) After run x sgroup, I got the NiO1.struct file as,

```
NiO1
F   LATTICE,NONEQUIV.ATOMS:  5 225 Fm-3m
MODE OF CALC=RELA unit=bohr
 15.854000 15.854000 15.854000 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=0.00005000 RMT=    2.3000   Z: 28.0
```

3) Then after init and using 1 k point and fix Rkmax equal to 5, I have modified inst file as,

```
Ni
Ar 3
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
```

4) For 4.5 ↑, 4 ↓ calculation, I have made NiO1.incup file as,

```
 7 1.00  0  NUMBER OF ORBITALS (EXCLUDING SPIN), SHIFT, IPRINT
1,-1,2             ( N,KAPPA,OCCUP)
2,-1,2             ( N,KAPPA,OCCUP)
2, 1,2             ( N,KAPPA,OCCUP)
2,-2,4             ( N,KAPPA,OCCUP)
3,-1,2             ( N,KAPPA,OCCUP)
3, 2,4             ( N,KAPPA,OCCUP)
3,-3,5             ( N,KAPPA,OCCUP)
```

Similarly for NiO1.incdn as,

```
 7 1.00  0  NUMBER OF ORBITALS (EXCLUDING SPIN), SHIFT, IPRINT
1,-1,2             ( N,KAPPA,OCCUP)
2,-1,2             ( N,KAPPA,OCCUP)
2, 1,2             ( N,KAPPA,OCCUP)
2,-2,4             ( N,KAPPA,OCCUP)
3,-1,2             ( N,KAPPA,OCCUP)
3, 2,4             ( N,KAPPA,OCCUP)
3,-3,4             ( N,KAPPA,OCCUP).....................
```

5) Removing impurity d states from valence states.
a) I did not understand, how to set linearization energy far above the Fermi level in wein2k files. Please tell me about
this. The default of my in1 file is,

```
WFFIL  EF=.3746787355   (WFFIL, WFPRI, ENFIL, 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
```

6) After removing the 8.5 electrons into the core, in2 file look like,

```
TOT            (TOT,FOR,QTL,EFG,FERMI)
  -9.00  167.50   0.50 0.05  1   EMIN, NE, ESEPERMIN, ESEPER0, iqtlsave
GAUSS    0.006      (GAUSS,ROOT,TEMP,TETRA,ALL      eval)
```

7) After Scf calculations
a) grepline :fer 'NiO1.scf' 1 gives FER : F E R M I – ENERGY(GAUSS-.M.)= 0.3746787355 (Is it in Ry)
b) grepline :3dd001 'NiO1.scf' 2 | head -2 | tail -1 gives NiO1.scf::3DD001: 3D*   0.406614692 Ry
c) grepline ':3d 001' 'NiO1.scf' 2 | head -2 | tail -1 gives NiO1.scf::3D 001: 3D   0.421862130 Ry
d) ε 3d↑ energy is calculated as (4*0.406614692+5* 0.42186213)/9=0.41508503 Ry.

8) Similar procedure I have applied for 4.5 ↑, 3 ↓ calculation.
And found a) F E R M I - ENERGY(GAUSS-.M.)= 0.3981117023
b) 3dd001=0.339923029 Ry and 3d001=0.355725953 Ry
c) ε 3d↑ energy is (4*0.339923029+5*0.355725953)/9=0.348702431 Ry
Now using these values in F_{eff} =ε 3d↑(4.5 ↑, 4 ↓)-ε 3d↑(4.5 ↑, 3 ↓)-ε f (4.5 ↑, 4 ↓)+ε f (4.5 ↑, 3↓)=0.09 Ry.
However according to notes in wein2k, it should be 0.438 Ry. Please shed a light on this.