SIESTA Exercise: MnO, three different magnetic configurations

```
SystemName      Manganese Oxide AFM1  # [001] magnetic ordering
SystemLabel            MnO_AF1        # Short name for naming files
%block LatticeVectors
 0.50     0.50      0.0
-0.50     0.50      0.0
 0.0      0.0       1.00
%endblock LatticeVectors
%block AtomicCoordinatesAndAtomicSpecies
 0.00   0.00   0.00  1
 0.00   0.50   0.50  1
 0.0    0.50   0.0   2
 0.0    0.0    0.50  2
%endblock AtomicCoordinatesAndAtomicSpecies
%block DM.InitSpin       # Describe the initial magnetic order (on Mn only)
 1   +
 2   -
%endblock DM.InitSpin

siesta: iscf   Eharris(eV)      E_KS(eV)   FreeEng(eV)   dDmax  Ef(eV)
siesta:    1    -2091.4756    -2068.7533    -2068.7533  0.1524 -0.2680
  (...)
siesta:   15    -2091.1220    -2091.1229    -2091.1229  0.0001 -2.8058

mulliken: Spin UP
Species: Mn
Atom  Qatom  Qorb
               4s      4s      3dxy    3dyz    3dz2    3dxz    3dx2-y2 3dxy
               3dyz    3dz2    3dxz    3dx2-y2 4Ppy    4Ppz    4Ppx
   1  5.588   0.055   0.240   0.990   0.989   0.960   0.989   0.958  -0.010
            -0.016   0.025  -0.016   0.025   0.131   0.137   0.131
   2  0.744  -0.039   0.223   0.034   0.044   0.089   0.044   0.092  -0.006
            -0.007  -0.005  -0.007  -0.004   0.097   0.092   0.097
Species: O
(...)
mulliken: Qtot =       13.000
mulliken: Spin DOWN
Species: Mn
Atom  Qatom  Qorb
               4s      4s      3dxy    3dyz    3dz2    3dxz    3dx2-y2 3dxy
               3dyz    3dz2    3dxz    3dx2-y2 4Ppy    4Ppz    4Ppx
   1  0.744  -0.039   0.223   0.034   0.044   0.090   0.044   0.092  -0.006
            -0.007  -0.005  -0.007  -0.004   0.097   0.092   0.097
   2  5.588   0.055   0.240   0.990   0.989   0.961   0.989   0.958  -0.010
            -0.016   0.025  -0.016   0.025   0.131   0.137   0.131
Species: O
(...)
mulliken: Qtot =       13.000
```

SIESTA Exercise: MnO, three different magnetic configurations

```
SystemName      Manganese Oxide AFM2  # [111] magnetic ordering
SystemLabel            MnO_AF2        # Short name for naming files
%block LatticeVectors
 1.00     0.50      0.50
 0.50     1.00      0.50
 0.50     0.50      1.00
%endblock LatticeVectors
%block AtomicCoordinatesAndAtomicSpecies
 0.00   0.00   0.00  1
 1.00   1.00   1.00  1
 0.50   0.50   0.50  2
 1.50   1.50   1.50  2
%endblock AtomicCoordinatesAndAtomicSpecies
%block DM.InitSpin       # Describe the initial magnetic order (on Mn only)
 1   +
 2   -
%endblock DM.InitSpin

siesta: iscf   Eharris(eV)      E_KS(eV)   FreeEng(eV)   dDmax  Ef(eV)
siesta:    1    -2091.8778    -2087.1119    -2087.1119  0.9320 -3.3034
(...)
siesta:   14    -2091.2824    -2091.2835    -2091.2835  0.0001 -3.2644

mulliken: Spin UP
Species: Mn
Atom  Qatom  Qorb
               4s      4s      3dxy    3dyz    3dz2    3dxz    3dx2-y2 3dxy
               3dyz    3dz2    3dxz    3dx2-y2 4Ppy    4Ppz    4Ppx
   1  5.512   0.050   0.213   0.991   0.991   0.956   0.991   0.958  -0.016
            -0.016   0.021  -0.016   0.021   0.123   0.123   0.123
   2  0.826  -0.044   0.246   0.040   0.041   0.115   0.041   0.115  -0.007
            -0.007  -0.007  -0.007  -0.007   0.103   0.103   0.103
Species: O
(...)
mulliken: Qtot =       13.000
mulliken: Spin DOWN
Species: Mn
Atom  Qatom  Qorb
               4s      4s      3dxy    3dyz    3dz2    3dxz    3dx2-y2 3dxy
               3dyz    3dz2    3dxz    3dx2-y2 4Ppy    4Ppz    4Ppx
   1  0.826  -0.044   0.246   0.040   0.041   0.115   0.041   0.115  -0.007
            -0.007  -0.007  -0.007  -0.007   0.103   0.103   0.103
   2  5.512   0.050   0.213   0.991   0.991   0.956   0.991   0.958  -0.016
            -0.016   0.021  -0.016   0.021   0.123   0.123   0.123
Species: O
(...)
mulliken: Qtot =       13.000
```

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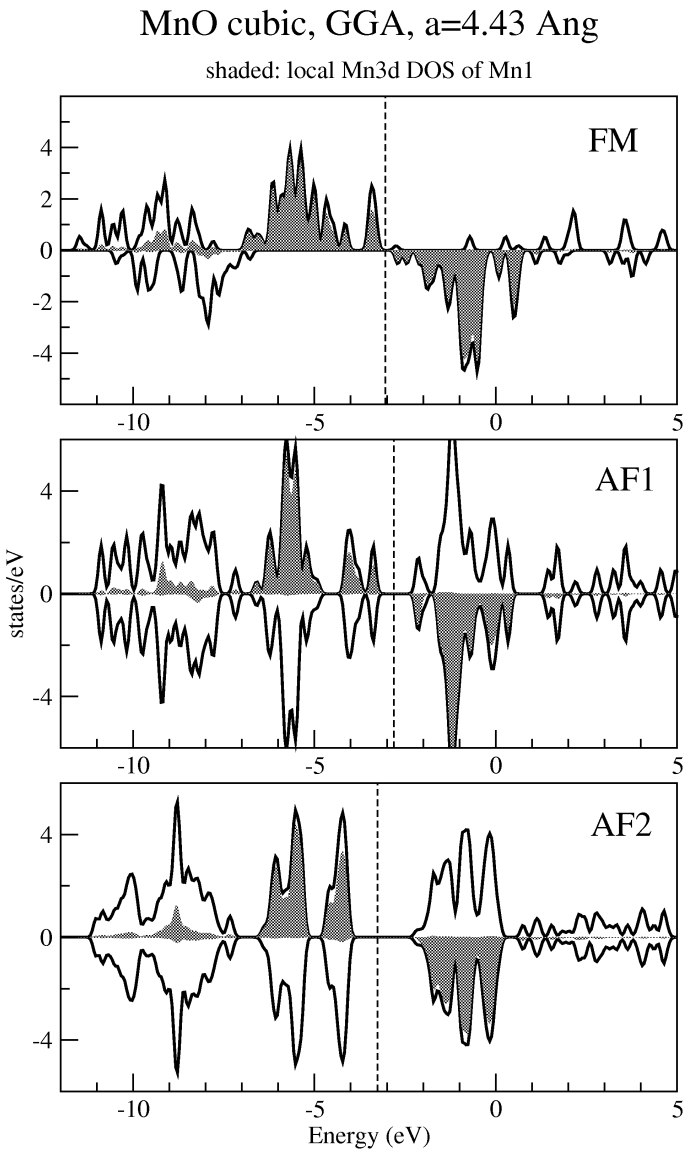


Left figure:

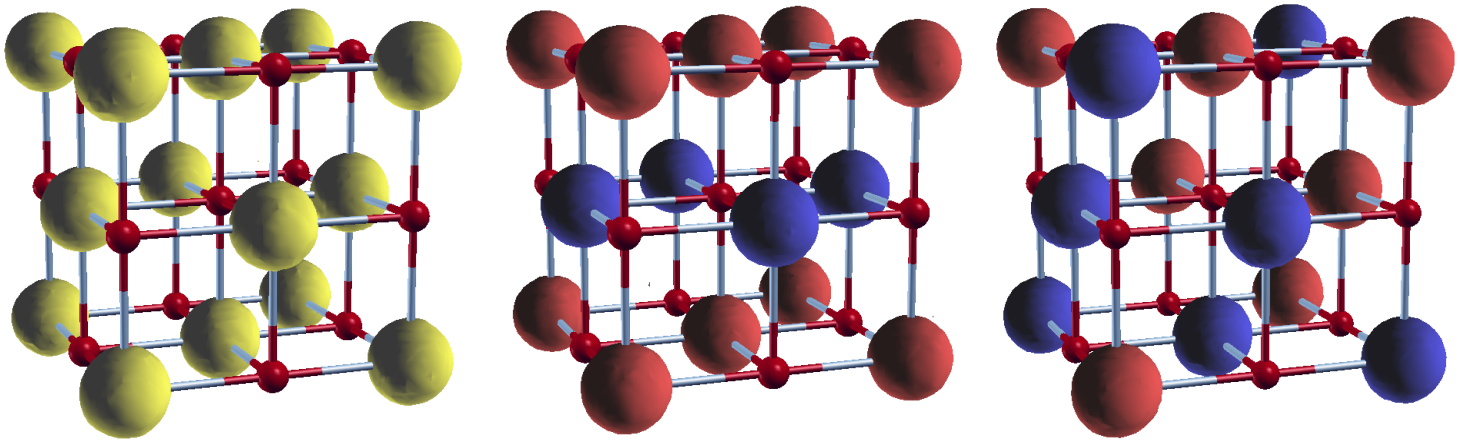
Spin-resolved
local (at Mn site) and total (per unit cell) densities of states.

Bottom figure:

Spatial magnetic density (levels ± 0.2) shown by different colours.

Think why the surfaces are so spherical around each Mn atom.

Try to identify t_{2g} and e_g states in the occupied part of the Mn3d DOS of AF2 structure, calculate and visualize LDOS separately for these two groups of states.



FM AF1 AF2