Antiferromagnetic calculations (w2web)

- **Antiferromagnetism: bcc Cr \( (a_0=2.885 \text{ Å}) \) (use 5000k, -cc 0.001)
  - try 2 different calculations:
    - ferromagnetic solution (bcc cell with 1 Cr)
    - antiferromagnetic calculation (P cell with Cr1 and Cr2 (at 0.5,0.5,0.5))
    - Before you initialize, run instgen_lapw and with up/dn for the two Cr atoms
    - for afminput your symmetry operation is “identity+(0.5,0.5,0.5)” (you need to go to individual mode)

- is FM or AFM Cr more stable? (::ENE)

- is FM stable at all? check moments (MMI001: what “means” 0.000x ???)

- plot AFM spin-densities in the (110) planes
  - do lapw1/2 for both spins
  - observe “spatial localization”
  - \( t_{2g} \)-asymmetry
  - negative spin-density in interstitial
    - where does it come from?
    - compare :QTLxxx
NiO: NaCl structure, A-type AFM along [111] (in command line mode)

- mkdir NiO; cd NiO; makestruct; cp init.struct NiO.struct
  - R-cell: 5.605236 5.605236 27.459934 bohr; angles: 90,90,120
  - 3 non-equivalent atoms: Ni1 (0,0,0), Ni2 (0.5,0.5,0.5), O ±(.25,.25,.25). View and “understand” the “NaCl” structure (Xcrysden)

- instgen_lapw -ask: select up,dn,nonmagnetic for the 3 atoms
- init_lapw -b -sp -numk 100

**GGA calculations:**
- runsp_lapw; save_lapw NiO_gga

**GGA+U calculations:**
- cp $WIENROOT/SRC_templates/case.inorb NiO.orb (and the same for case.indm)
  - (these templates are already for NiO, otherwise you have to edit them properly)
- runsp -orb; save_lapw NiO_gga_u

**GGA+SO calculations:**
- restore_lapw NiO_gga; initso_lapw
  - (M=[111], no relativistic LOs, Emax=5.0, select spin-polarization and accept files)
- runsp -so; x lapwdm -up -so (and check the orbital moment :ORB001 in *scfdmup)
- save_lapw NiO_gga_so
LDA+U calculations

- **GGA+U+SO calculations**: 
  - runsp -so -orb; save_lapw NiO_gga_u_so
- **compare the gaps**: GAP (exp: 4eV): grepline :GAP "*scf" 1
- **compare spin moments**: MMI001
- **compare orbital moments for SO and SO+U calculations**: ORB001
- **calculate and compare DOS for GGA and GGA+U** (see shifts of Ni/O weights)
  - restore_lapw NiO_xxx
  - x lapw1 -up/dn (-orb); x lapw2 -qtl -up/dn
  - configure_int (and select total, Ni1, Ni2, O-tot)
  - x tetra -up/dn
  - dosplot2 -up

- **try a TB-mBJ calculation for NiO** (starting from GGA) follow instructions given in mBJ exercises or F. Tran's lecture) and compare gap/DOS
FIG. 2 (color online). DOS of NiO. The vertical bars indicate the end of the fundamental band gap which starts at $E = 0$ eV. The panels labeled “Expt.” show photoelectron [25] (upper panel) and XES [33] [lower panel, Ni (solid line) and O (dashed line) spectra] measurements.

from Tran, Blaha, PRL 102, 226401 (2009)