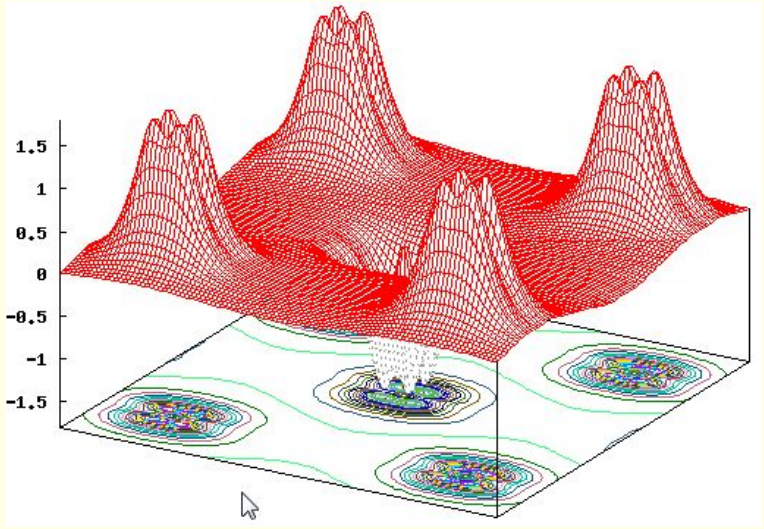
Antiferromagnetic calculations (w2web)

- Antiferromagnetism: bcc Cr (a_0=2.885 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: GGA+U/spin-orbit/mBJ calc. (command line)

- 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*

NiO cont...

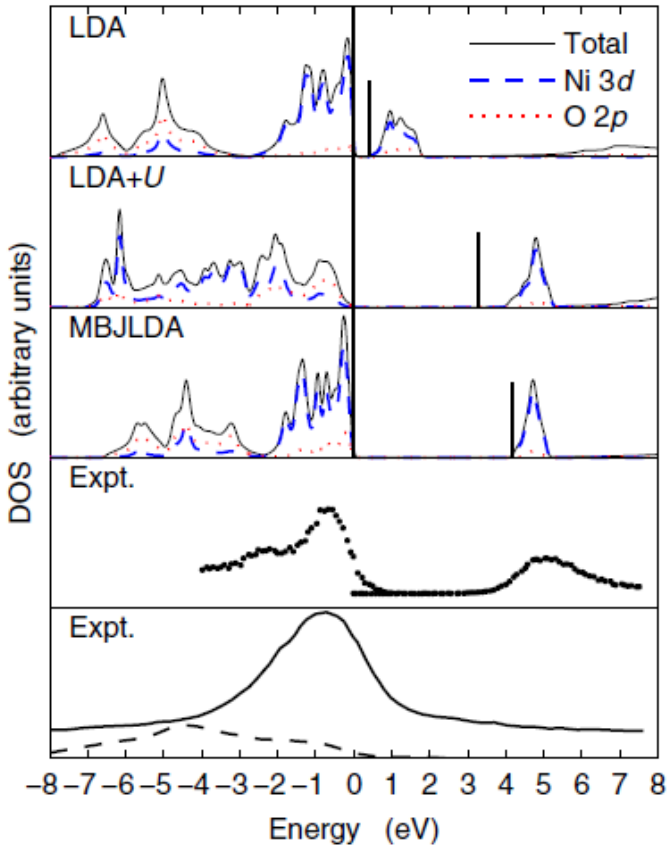


FIG. 2 (color online). DOS of NiO. The vertical bars indicate the end of the fundamental band gap which starts at $E = 0$ eV. The panels labeled "Expt." show photoelectron [25] (upper panel) and XES [33] [lower panel, Ni (solid line) and O (dashed line) spectra] measurements.

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

GGA+U