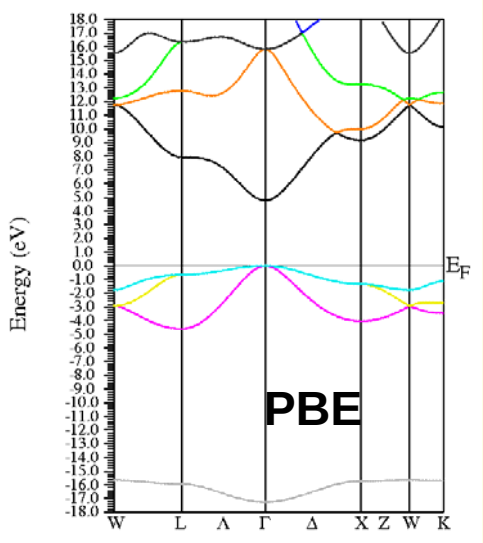
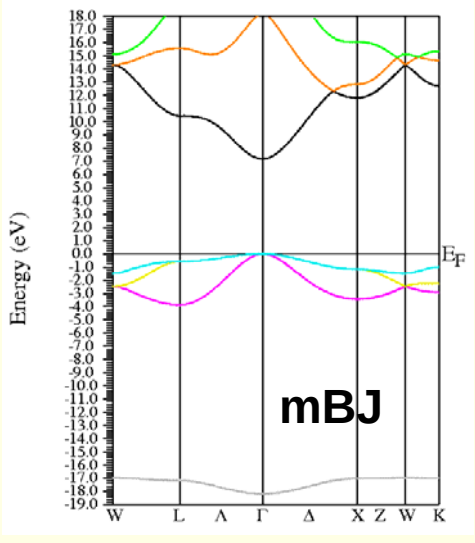
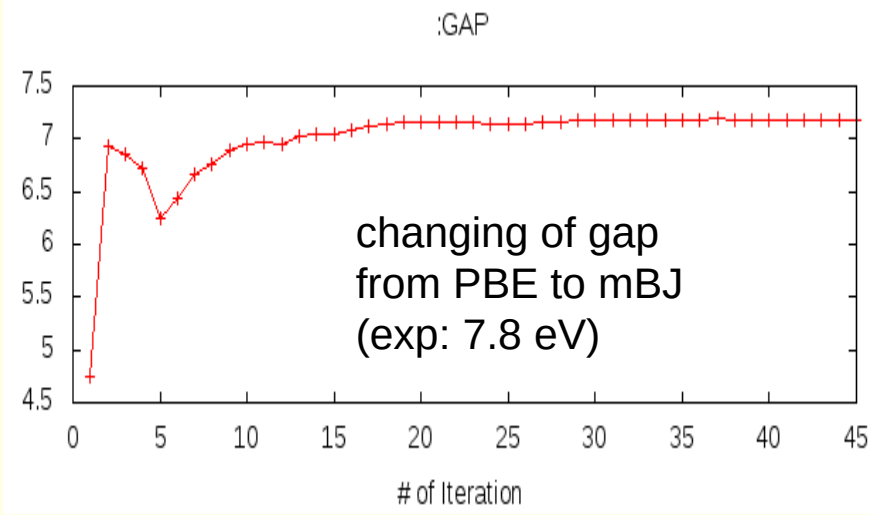
Band gaps of MgO in various approximations

- MgO (NaCl, a=7.96 bohr; default initialization; scf-cycle)
  - *PBE: check the gap (:GAP from "anaylysis"),*
    - plot a band structure in PBE (E-range from -19 to 18 eV)
  - *TB-mBJ:*
    - save the PBE calculation, execute:
      - init_mbj_lapw (in utils) „phase 1" of the initialization (see also in the UG 4.5.9)
      - run_lapw -NI -i 1
      - rm *.bro*
      - init_mbj_lapw „phase 2", use original mBJ parameters
    - run scf cycle (note, it may not converge in 40 cycles, submit another run with -NI option)
    - monitor the change of the :GAP
    - plot a band structure (fcc) and compare with PBE







Exercise 7: continued ...

- Perform a hybrid-DFT calculation using YS-PBE0
  - create a new case, perform a PBE calculation and save the results.
  - the setup for hybrid-calculations can be made in w2web (Utils/init_hf_lapw), or in a terminal-window using „init_hf_lapw“. (More details are given in the UG 4.5.8)
    - Select NBAND=12 (case.inhf)
    - and a 4x4x4 / 4x4x4 k-point mesh (no reduction)
  - scf cycle with **-hf -p -scratch ./** (insert 4 lines with **1:localhost** into **.machines**)
    - we do this in k-parallel since it will take more time, alternatively we could also use a „reduced“ hf-k-mesh, see UG
  - monitor the change of the :GAP and compare it with mBJ and exp. gaps (only every 2nd value is from HF !)
  - plot a band structure:
    - only the k-mesh selection can be done in w2web, then open a terminal and change into the proper directory
    - run_bandplothf_lapw -p
    - cp $WIENROOT/SRC_templates/case.insp case.insp (insert E_F and increase the plotting energy range).
    - x spaghetti -hf -p