Mg K-XANES in MgO

- MgO (NaCl structure, a=7.96 bohr; default initialization with 1000 k-points; scf-cycle)
  - XSPEC task: larger EMAX in MgO.in1; select in MgO.inx: Mg-K ABS from 0-30 eV, vary broadening)
- Supercells: MgO 2x2x2 FCC-supercell for core-hole simulation
  - create new “session”, copy MgO.struct into new directory
  - x supercell; (specify proper struct-filename, 2x2x2, F-lattice)
  - cp supercell-struct file to correct name “case.struct”; “label” 1st atom (Mg → Mg1)
  - init_lapw (with 200k, RKmax=6.5)
  - edit case.inc (remove a core electron from 1st atom)
  - edit case.in2 (add one valence electron)
  - run_lapw (for bigger calc. use -it and compare timings for 1st and later iterations!)
  - edit case.in2 (remove extra valence electron)
  - XSPEC task for Mg-K XAS (see above)

![Graphs showing Mg-K XAS with and without core hole]

no core hole

Mg-K XAS

with core hole
Optical properties: fcc Al

- $a_0 = 4.05 \text{ Å}$
- init_lapw (use 165 IBZ k-points only!)
- run_lapw
- calculate optics (as described in the optics lecture, compare with the Al - Fig.)
  - calculate plasma frequency (case.outputjoint) and dielectric function
  - check your results with respect to k-mesh
    - x kgen (check for about 1000 and 4000 IBZ-points)
    - x lapw1
    - x lapw2 -fermi
    - x optic, x joint, x kram

Optical properties: fcc Ag and Au (both have $a_0 = 4.08 \text{ Å}$)

- compare optics without / with spin-orbit coupling (compare with RL)
  - do NREL (change RELA to NREL in case.struct) first, do the optics
  - do scalar-relativistic calc., do the optics
  - include spin-orbit: run_lapw -so (case.inso without RLOs since optic does not support RLOs; put large Emax in case.in1); optics
Ag and Au: a relativistic effect

DOS

absorption