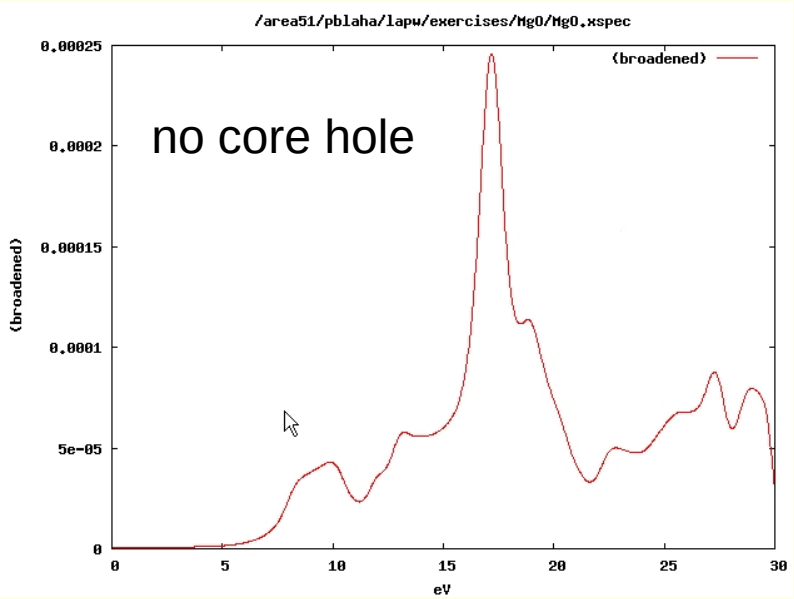
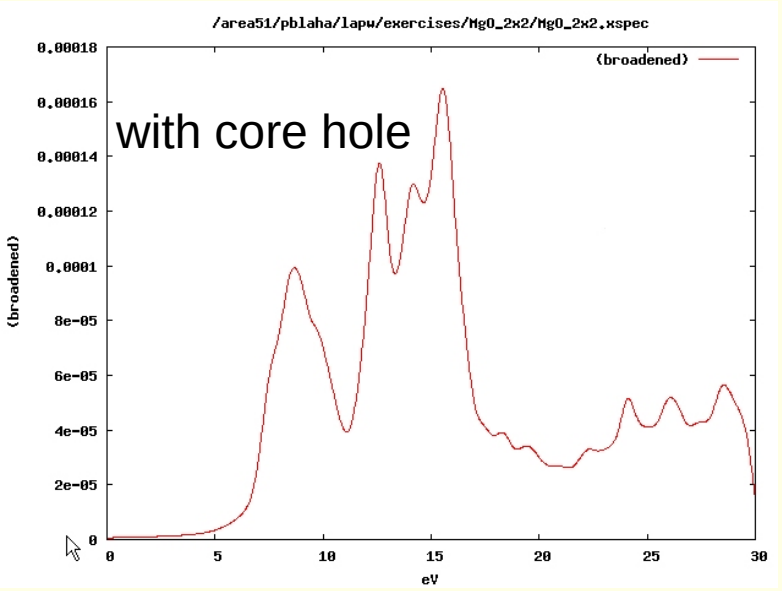
Mg K-XANES in MgO

- 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.inxs: 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)*



Mg-K XAS



optical properties: Al, Ag and Au

- Optical properties: fcc Al
  - *a_0=4.05 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 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