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Band structure calculations

Available calculations infrastructure

-8 computers with Pentium IV processor, hard disk 80 GB, 2 G RAM memory

Software:

-band structure calculation code SPRKKR Muenchen, 7.0 version, with *xband* graphical interface

-band structure calculation code TB-LMTO

Research topics

Band structure calculations

- Investigation of the electronic and magnetic properties in rare earth-3d transition metals, intermetallic compounds, permanent magnets, soft magnetic materials, half-metals.

Spectroscopy

- *ab initio* X-ray magnetic circular dichroism in absorption spectra. XAS spectroscopy.
- *ab initio* description of X-ray photoemission in the valence band.
- *ab initio* description of magnetic Compton scattering for pure metals and alloys.
- *ab initio* description of the electron-positron density of momentum. The analysis of the 2D-ACAR experimental spectra obtained from positron annihilation experiment.