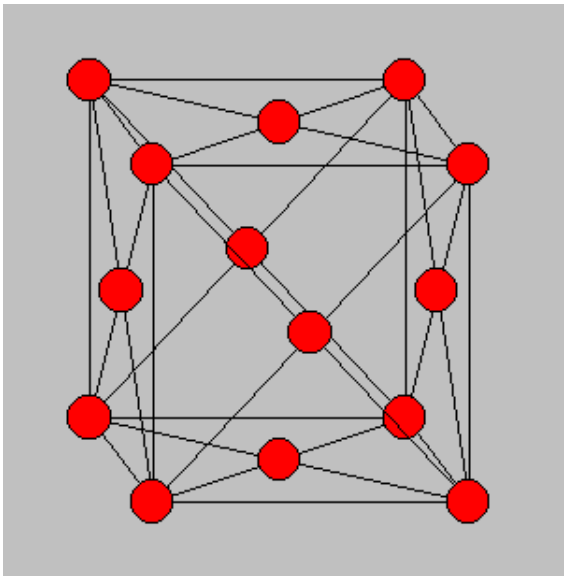
Bandstrukturmethoden Demo 2: Nickel-Kristall (fcc)

Bandstrukturrechnung mittels FP-LAPW WIEN2k-02

- **Kristallstruktur von metall. Ni → fcc**
- **Input für das WIEN-Programm**
- **Vorbereitung der Bandstrukturrechung (mit weiteren wichtigen Parametern).**
- **Die selbstkonsistente Bandstrukturrechnung**
- **Ergebnisse**
- **Variation von RKMAX = Größe der LAPW-Basis**



WIEN2k: An Augmented Plane Wave Plus Orbitals Program for Calculating Crystal Properties

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Elektronenstruktur (Z=28):

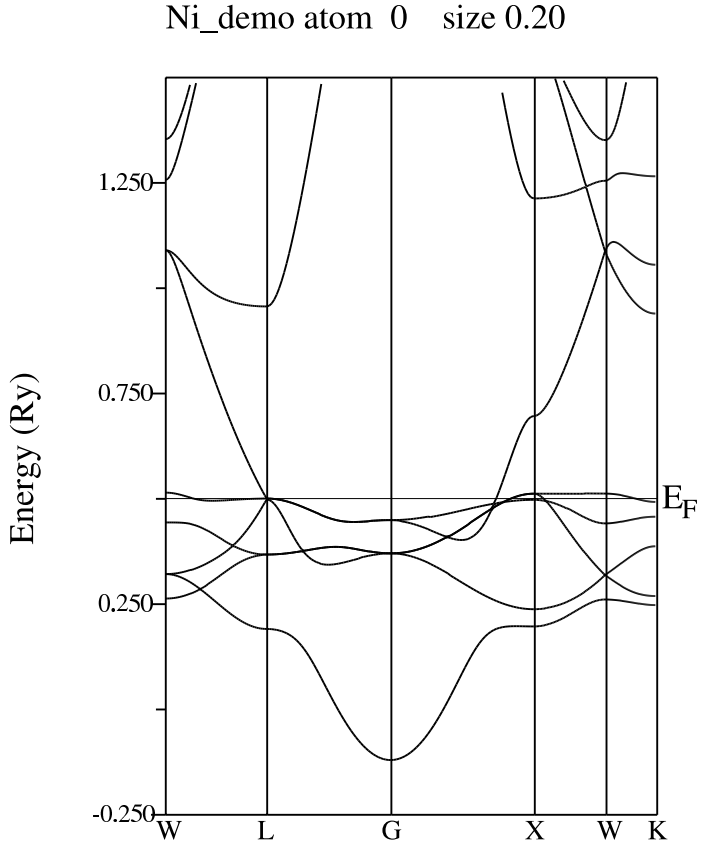
$$1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 3d^8\ \ 4s^2$$

oder

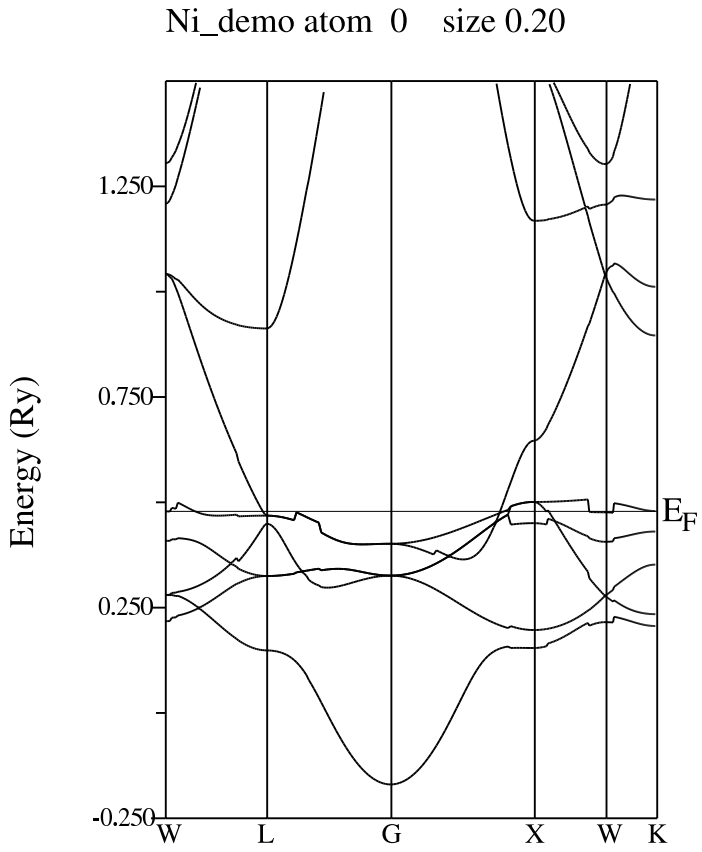
$$1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^6\ \ 3d^8\ \ 4s^2$$

- **Input für das WIEN-Programm: Ni_demo.struct**

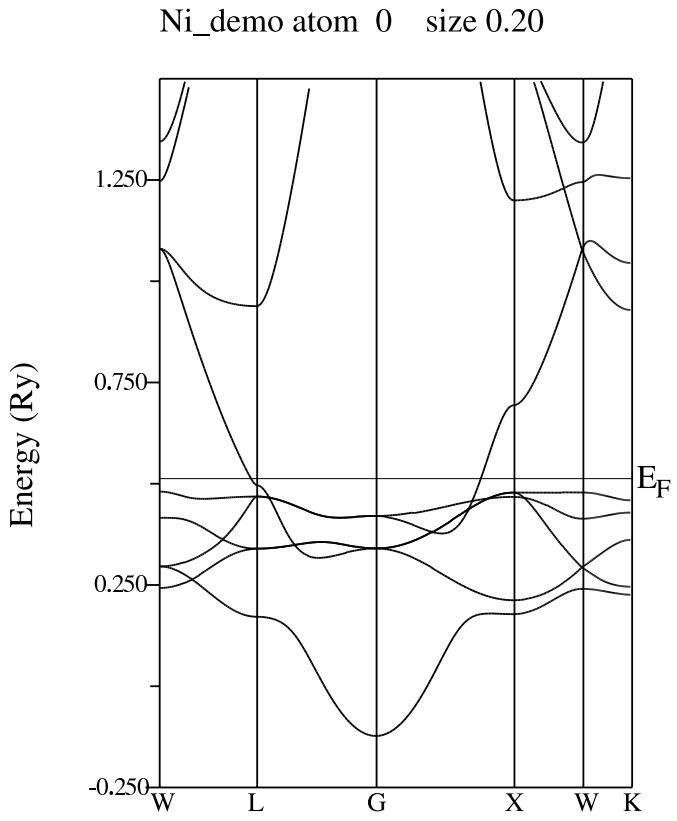
```
 FCC Ni
F    LATTICE,NONEQUIV.ATOMS: 1
MODE OF CALC=NREL
 6.7000    6.7000     6.7000
ATOM=  1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ni         NPT=  381  R0=.000050000 RMT=2.300000000  Z:28.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   0      NUMBER OF SYMMETRY OPERATIONS
```



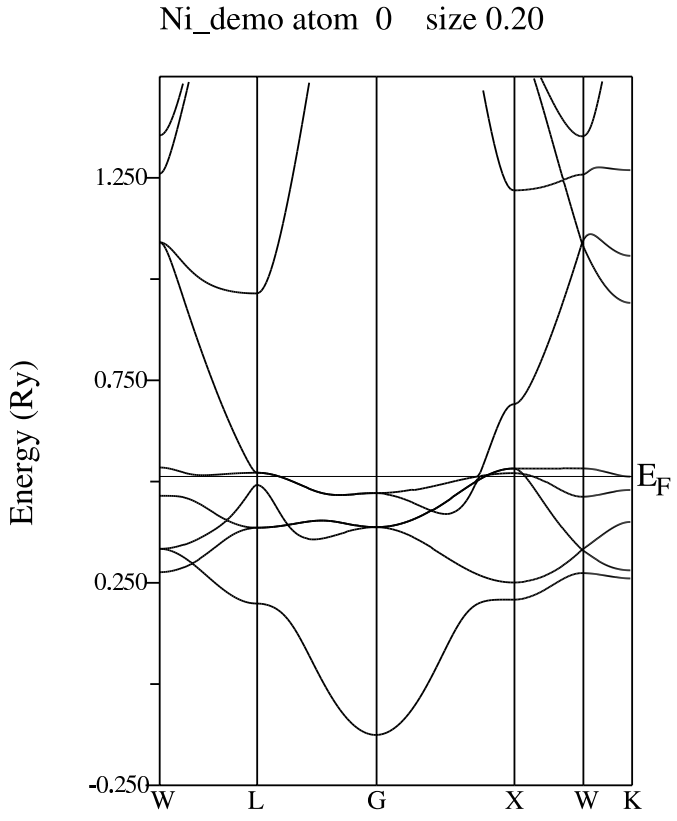
Nickel-Bandstruktur: RKMAX = 7.0



Nickel-Bandstruktur: RKMAX = 5.0



Nickel-Bandstruktur: spin-polarisiert UP



Nickel-Bandstruktur: spin-polarisiert DOWN

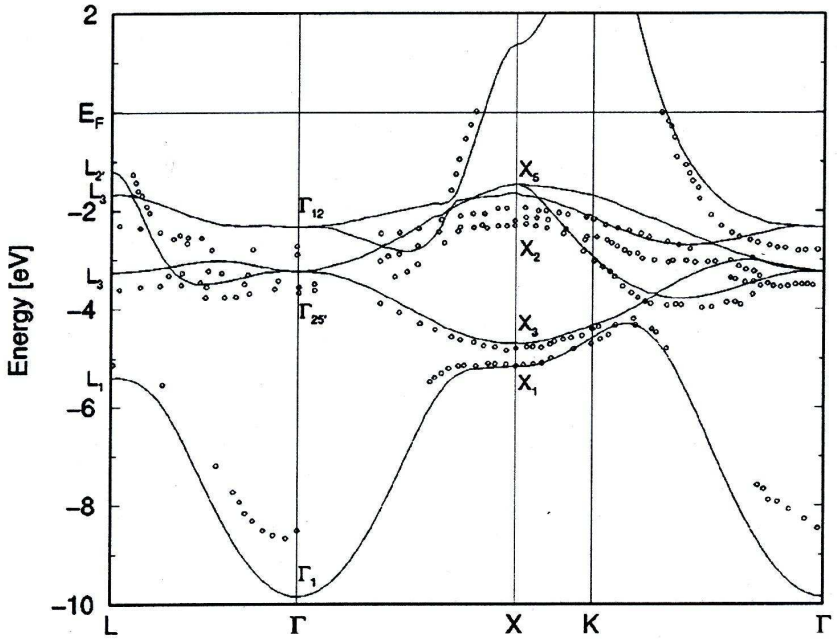


Figure 1: Bulk copper DFT-LDA band structure (solid line), compared with photoemission data (points).
Theory: Marini et al., Phys. Rev. B **64**, 195125 (2001),
experiment: Courths and Hüfner, Phys. Rep. **112**, 53 (1984).

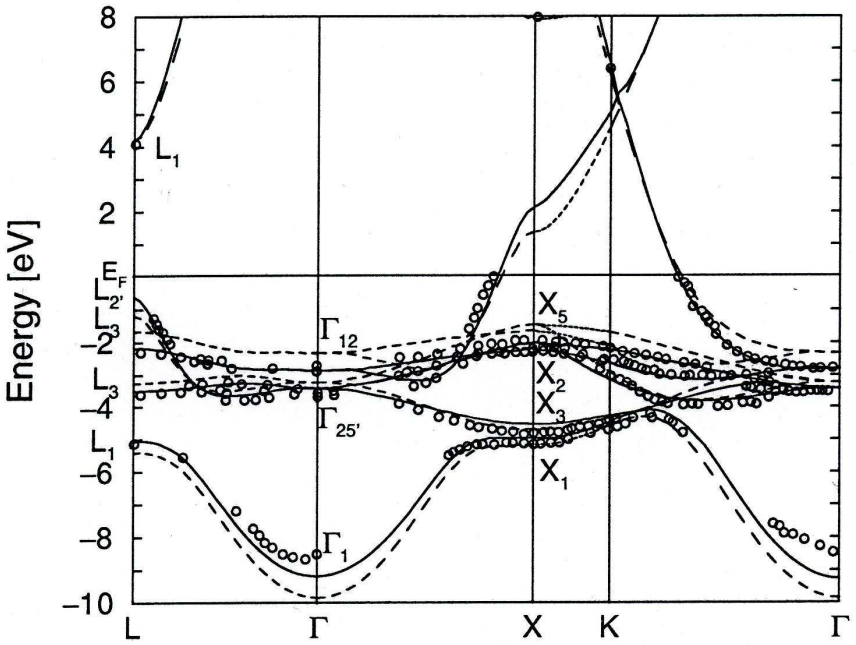


Figure 2: Solid line: GW results for the bulk copper band structure, compared with the DFT-LDA results (dashed line), and with experimental photoemission data.
Theory: Marini et al., Phys. Rev. Lett. **88**, 016403 (2002),
experiment: Courths and Hüfner, Phys. Rep. **112**, 53 (1984).