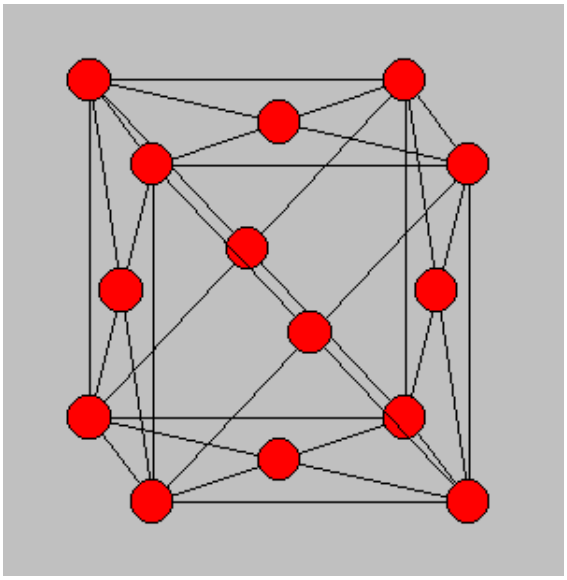
Bandstrukturmethoden Demo 1: Aluminimum-Kristall (fcc)

Bandstrukturrechnung mittels FP-LAPW WIEN2k-02

- **Kristallstruktur von metall. Al → fcc**
- **Input für das WIEN-Programm**
- **Vorbereitung der Bandstrukturrechung (mit weiteren wichtigen Parametern).**
- **Die selbstkonsistente Bandstrukturrechnung**
- **Ergebnisse**
- **evtl.: Parameter-Variationen**



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

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Inst. of Physical and Theoretical Chemistry, Vienna University of Technology

Elektronenstruktur (Z=13):

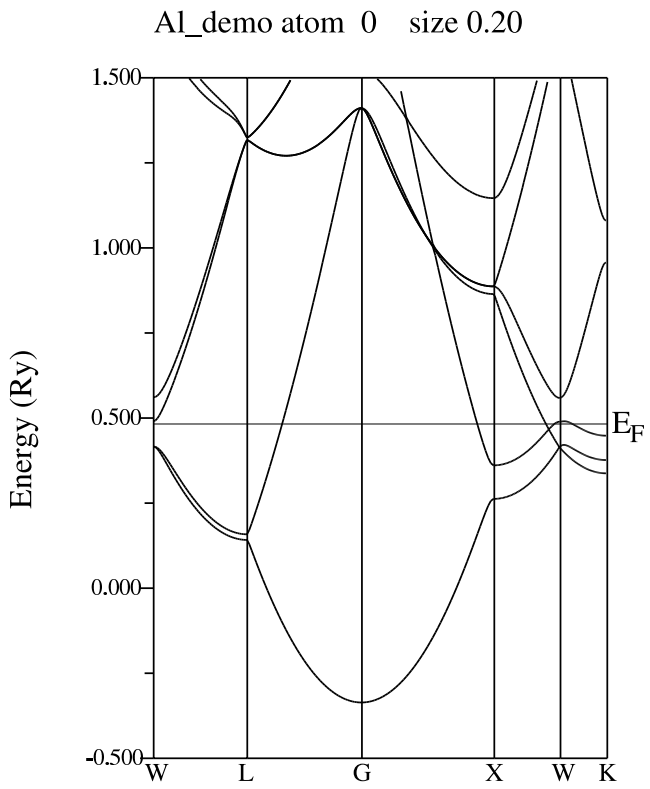
$$1s^2\ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^1$$

oder

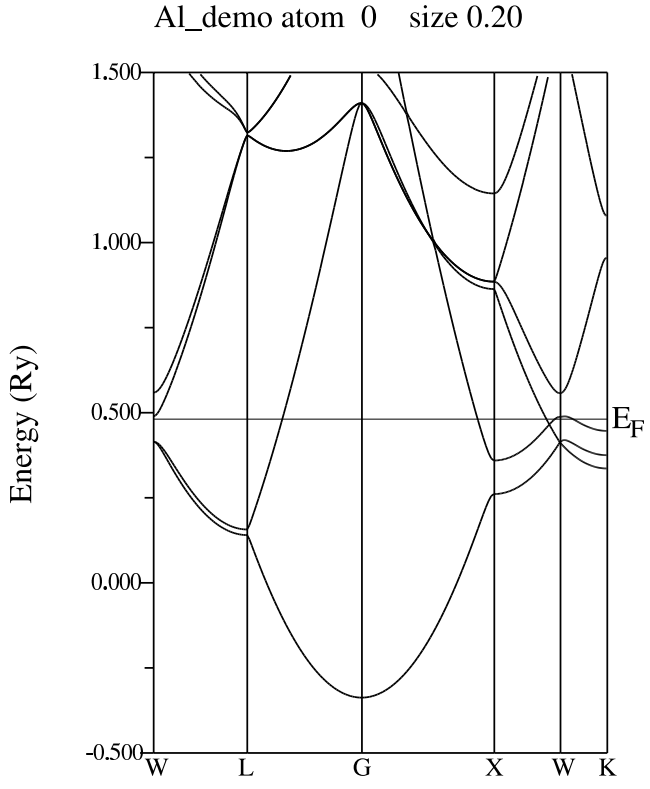
$$1s^2\ \ 2s^2\ \ 2p^6\ \ 3s^2\ \ 3p^1$$

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

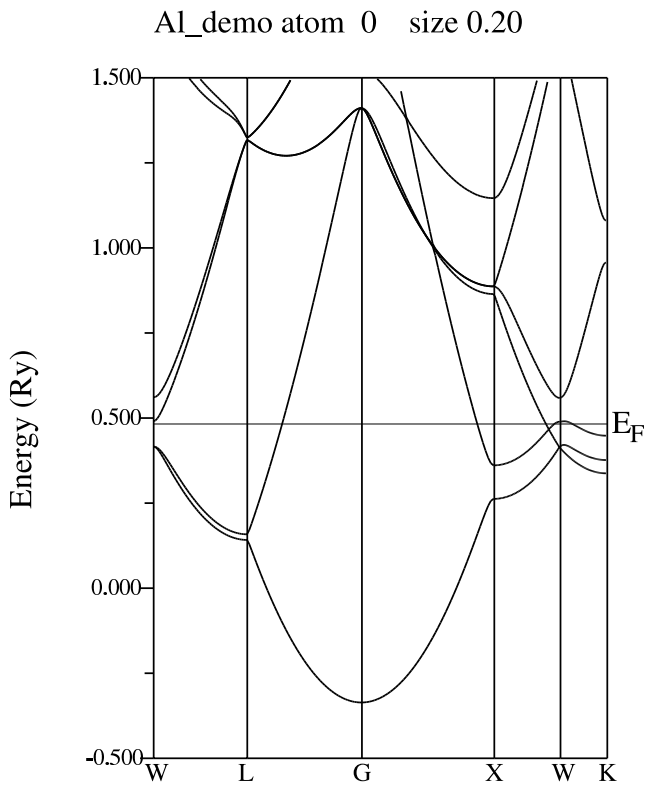
```
Al

F   LATTICE,NONEQUIV. ATOMS: 1

MODE OF CALC=NREL

  7.6517    7.6517    7.6517   90.0      90.0      90.0

ATOM=  1: X=0.00000000 Y=0.00000000 Z=0.00000000

          MULT= 1          ISPLIT= 2

Al         NPT=  381  R0=0.00005000 RMT=    2.7000   Z: 13.0

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
```



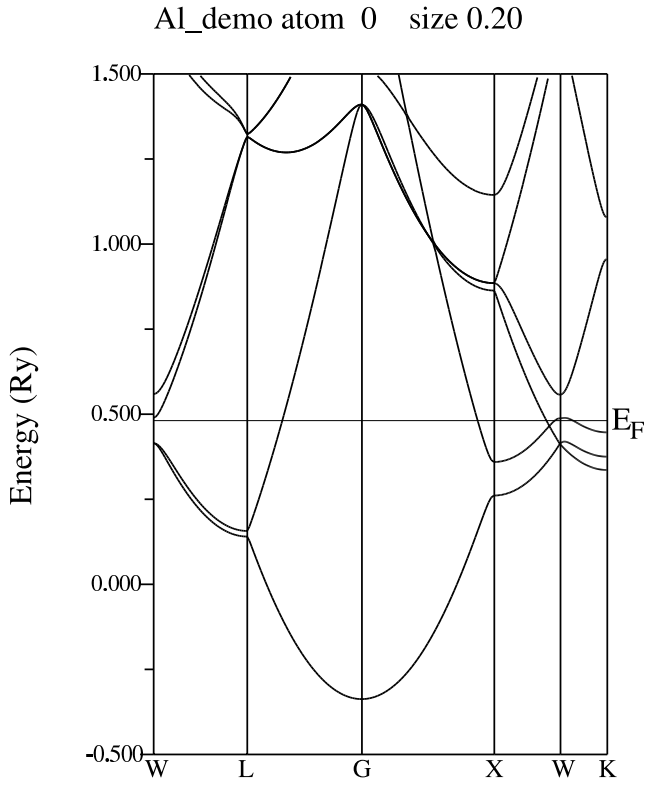
Aluminium-Bandstruktur: 2s und 2p als Bloch



Aluminium-Bandstruktur: 2s und 2p als Core



Aluminium-Bandstruktur: GGA



Aluminium-Bandstruktur: LSDA