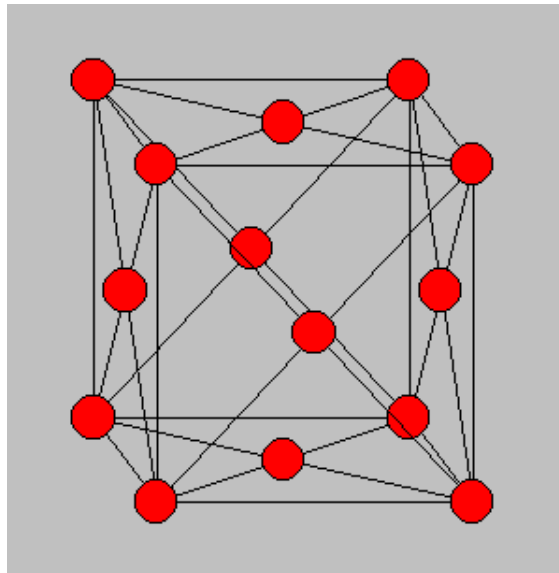


Bandstrukturmethoden Demo 1: Aluminium-Kristall (fcc)

Bandstrukturrechnung mittels FP-LAPW WIEN2k-02

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



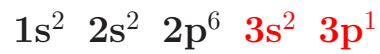
**WIEN2k: An Augmented Plane Wave Plus Orbitals
Program for Calculating Crystal Properties**

P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka,
J. Luitz,
Inst. of Physical and Theoretical Chemistry,
Vienna University of Technology

Elektronenstruktur (Z=13):



oder



- 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

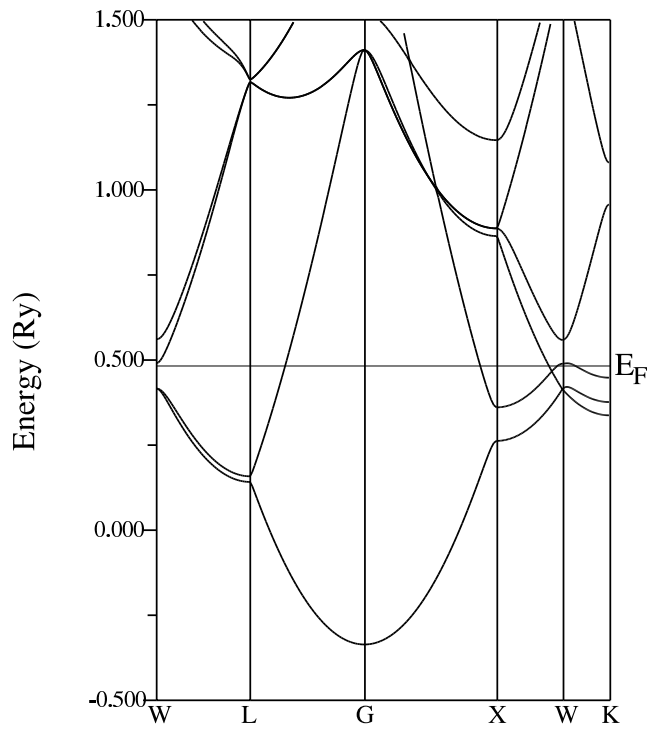
MULT= 1 ISPLIT= 2

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

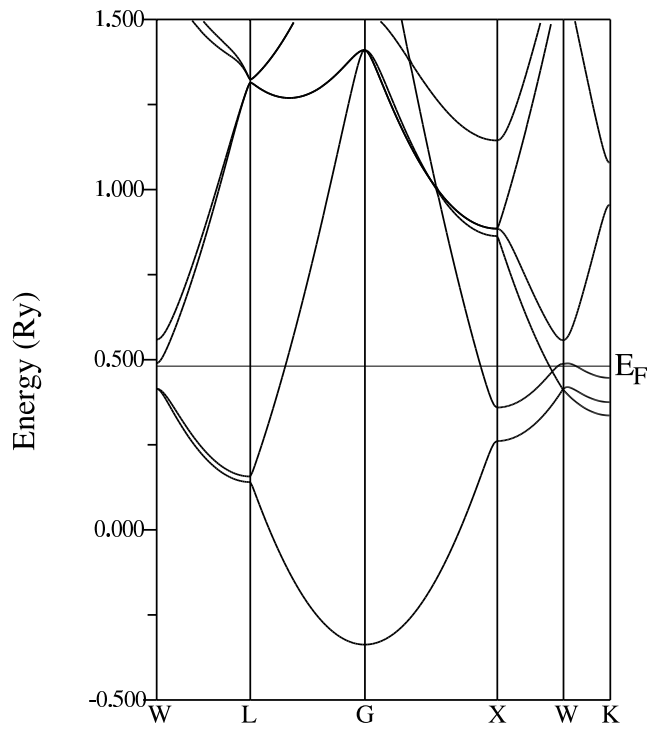
0 NUMBER OF SYMMETRY OPERATIONS

Al_demo atom 0 size 0.20



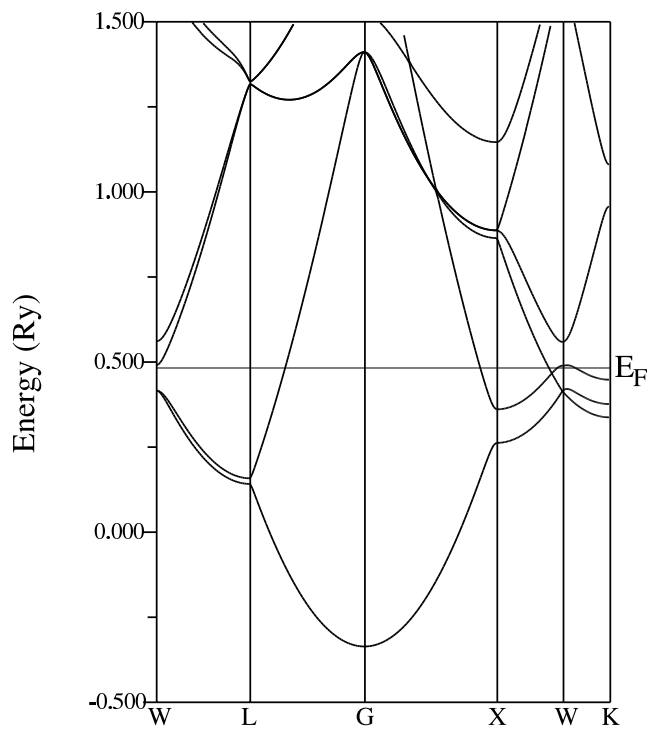
Aluminium-Bandstruktur: 2s und 2p als Bloch

Al_demo atom 0 size 0.20



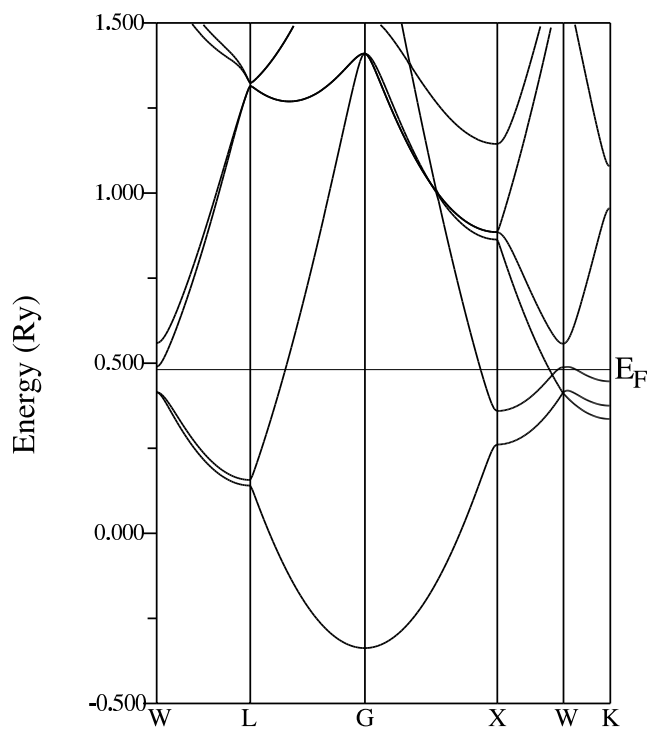
Aluminium-Bandstruktur: 2s und 2p als Core

Al_demo atom 0 size 0.20



Aluminium-Bandstruktur: GGA

Al_demo atom 0 size 0.20



Aluminium-Bandstruktur: LSDA