Silicon

Bandstructurcalculation with WIEN2k

Materialparameter

Cristallisation: Diamond

Z: 14

Latticeconstante: 10.26 Bohr

Inputparameter

Muffin-tin radius: 2.2

NPT: 781

Gauss for DOS: 0.003

Calculation

Exchange-Correlation Potential: Generalized Gradient Approximation

Energy which separates core and valenz states: -6.0 Ry

k_{max}: 8.00

k-Points in the whole BZ: 20000

No spinpolarized calculation

Non relativistic calculation

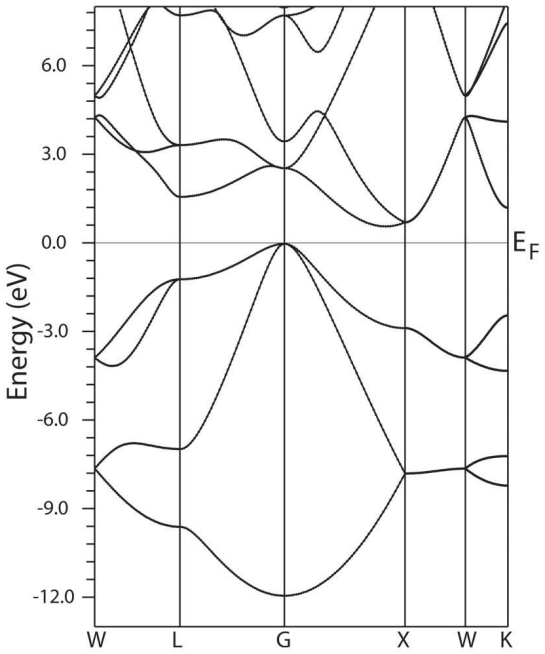
Outcome

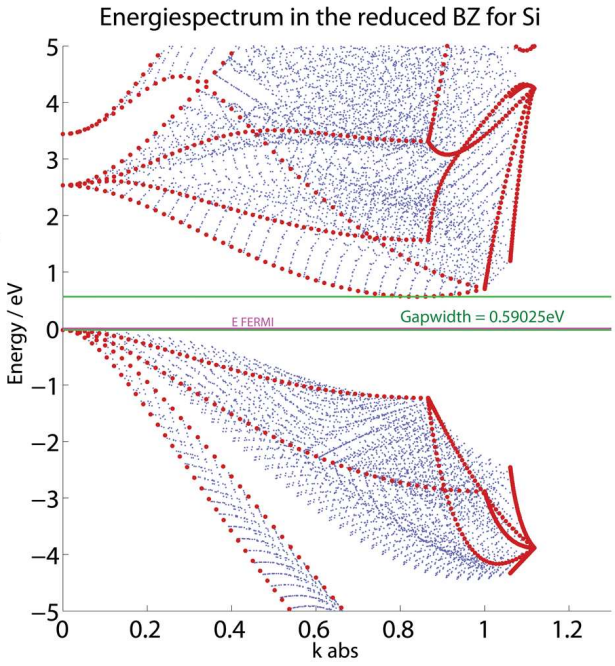
E_{Fermi}: 0.39 Ry

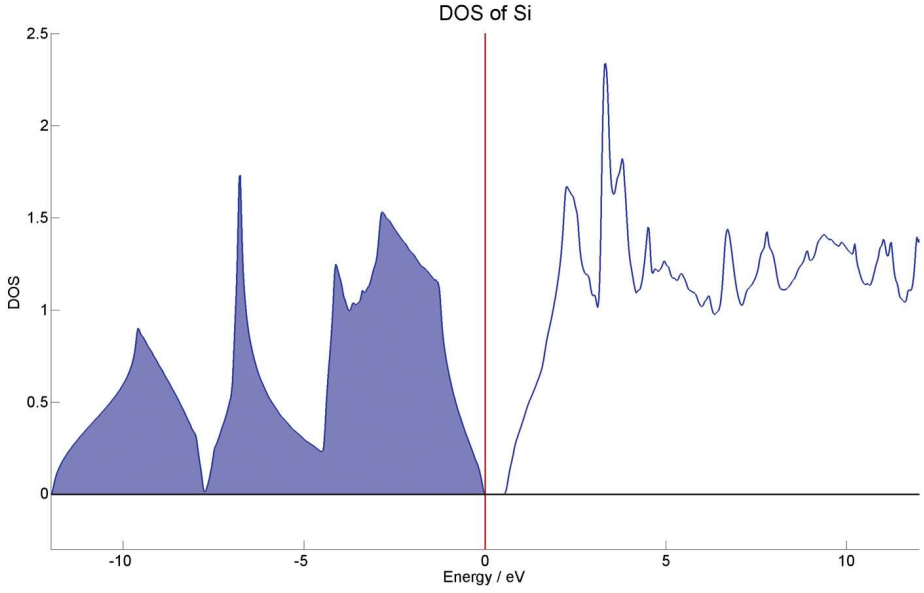
Gapwidth: 0.59 eV

Pictures upleft: Dispersionrelation; upright: Energy to k_{abs} in the whole BZ (red: WLGXWK-way); botton: DOS

Katrin Unger; Graz, 29. April 2011


6.0
3.0
0.0
-3.0
-6.0
-9.0
-12.0
Energy (eV)
E_F
W
L
G
X
W
K


Energiespectrum in the reduced BZ for Si
Energy / eV
E FERMI
Gapwidth = 0.59025eV
k abs


DOS of Si
DOS
Energy / eV