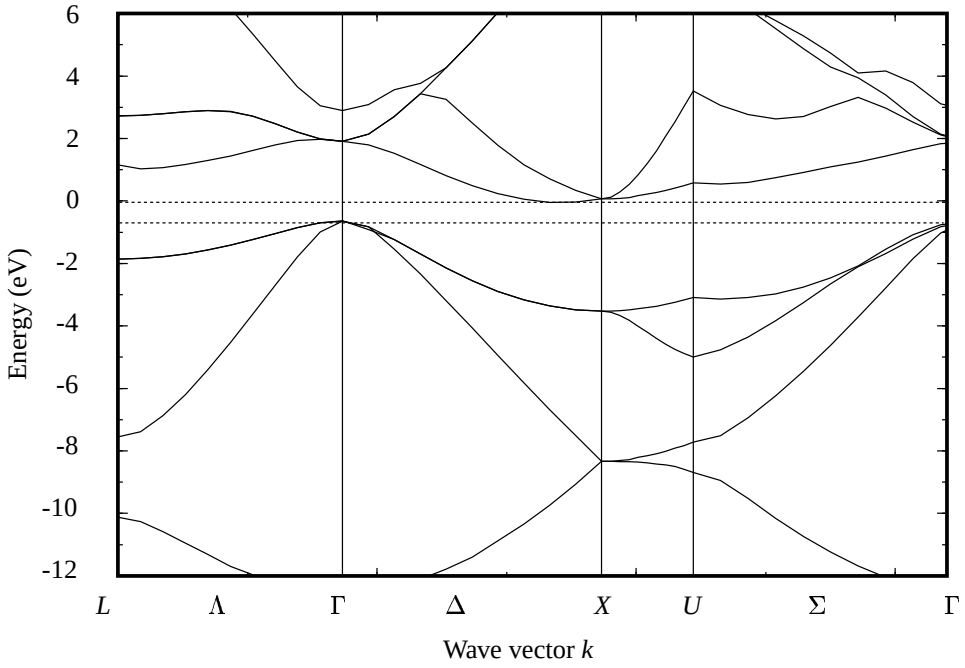

Figure 10.9. Energy bands of silicon, as calculated with plane-wave pseudopotential code of Stumpf and Scheffler (1994). The calculation assumes that silicon adopts the diamond structure, with a lattice spacing of 5.43 Å, and uses about 150 plane waves. Detailed features, such as the band gap, do not compare well with the more sophisticated calculations and experimental measurements in Figure 23.16.

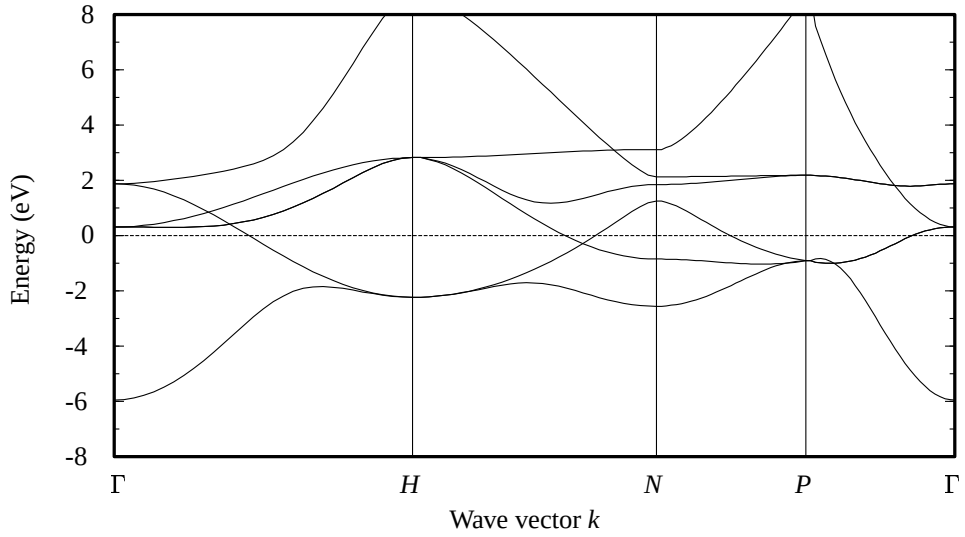

Figure 10.10. Energy bands of vanadium, as calculated with the plane-wave pseudopotential code VASP of Kresse and Hafner (1994) and Kresse and Furthmüller (1996). The calculation uses the fact that vanadium adopts the bcc structure, and it requires about 1000 plane waves. The location of the Fermi level in the midst of the complicated *d* bands is characteristic of the transition metals.