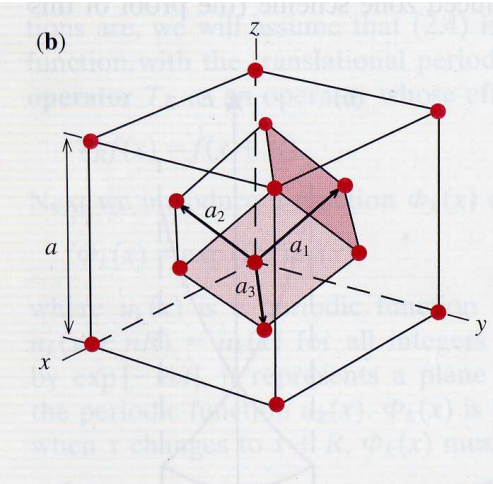
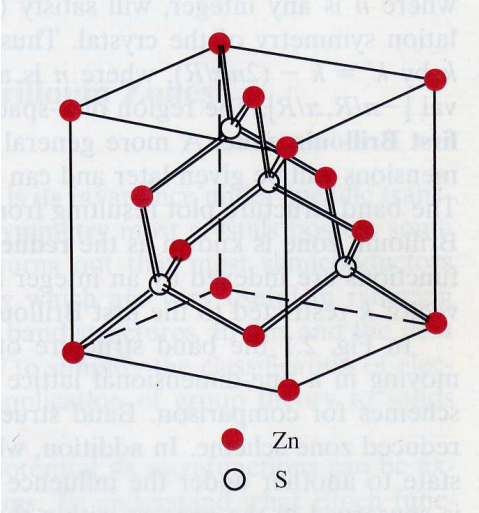
Examples of Real Band Structures

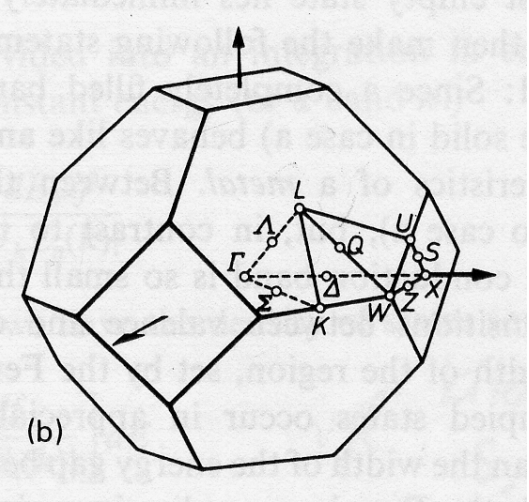
Restricted here to Zincblende semiconductors including the special case of the diamond structure (C, Si, Ge).



Lattice



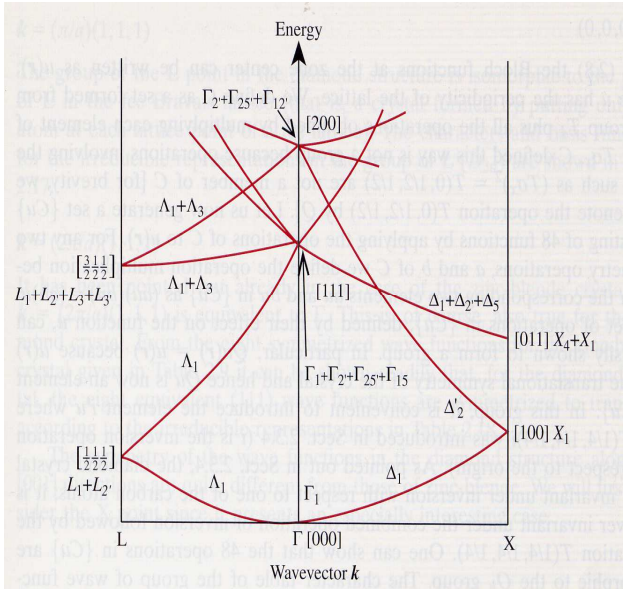
Basis of atoms

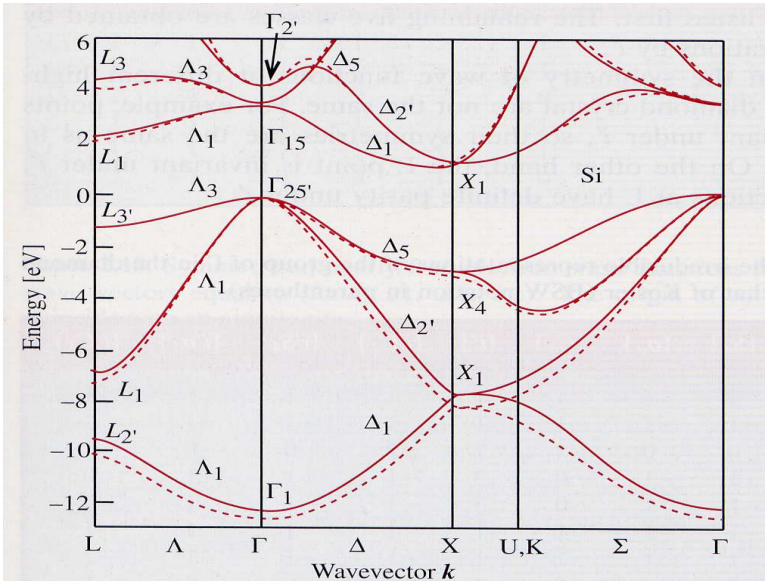


(1.) Brillouin zone

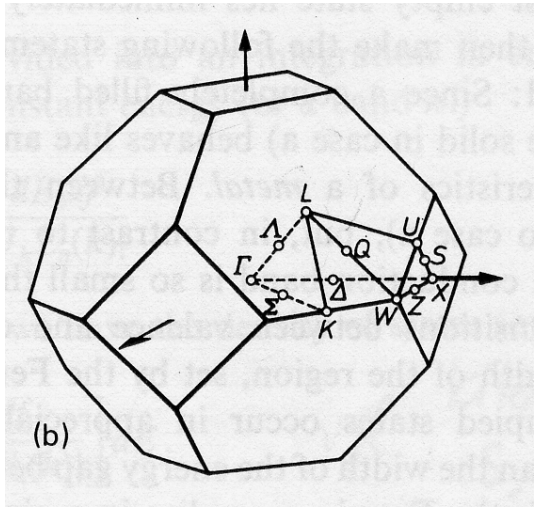
NFE and Real Band Structure

Restricted here to Zincblende semiconductors including the special case of the diamond structure (C, Si, Ge).

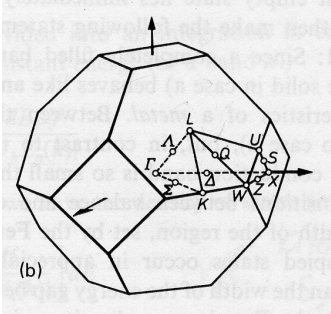




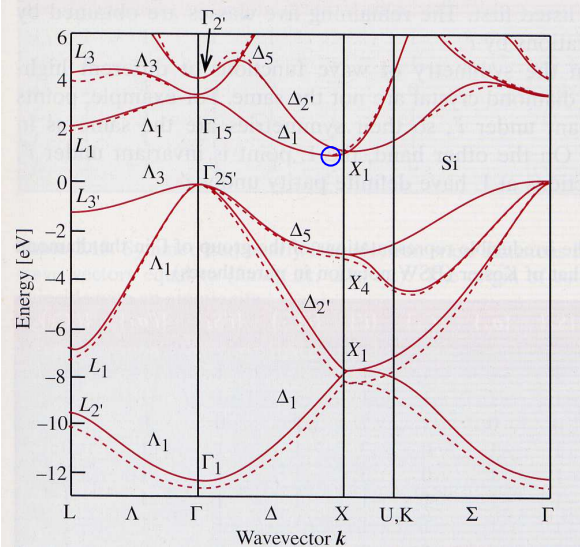
with
local
non local
pseudo-potential



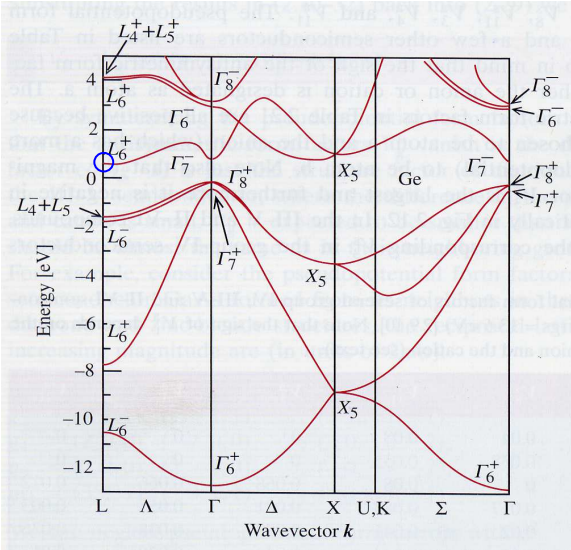
- For semiconductors, strong splitting creates a band gap!
- Symbols are symmetry notations of the wave functions.
- At symmtery lines/points, degeneracy can persist.



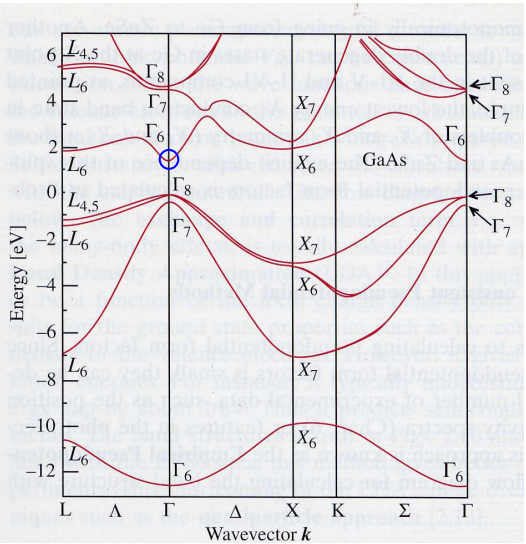
Comparison along the Periods of the PSE



indirect…….



indirect…….



direct band gap

bands 2 and 3/4 at Γ:

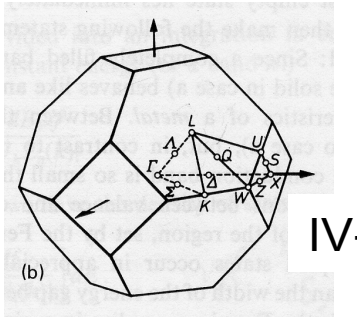
degenerate

non-degenerate

non-degenerate

spin-orbit splitting ~ z !

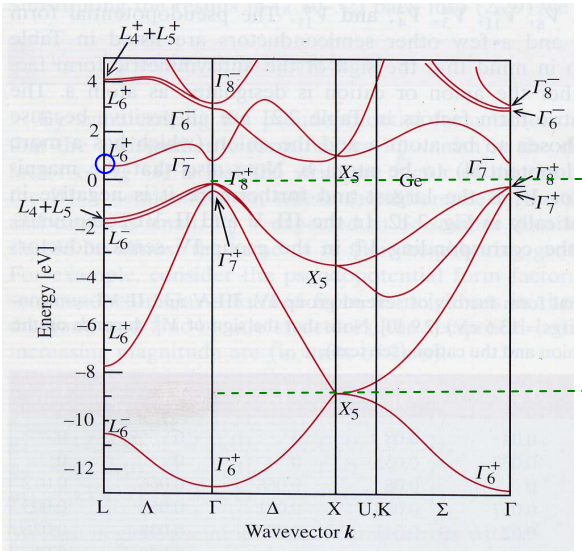
Increase Ionicity

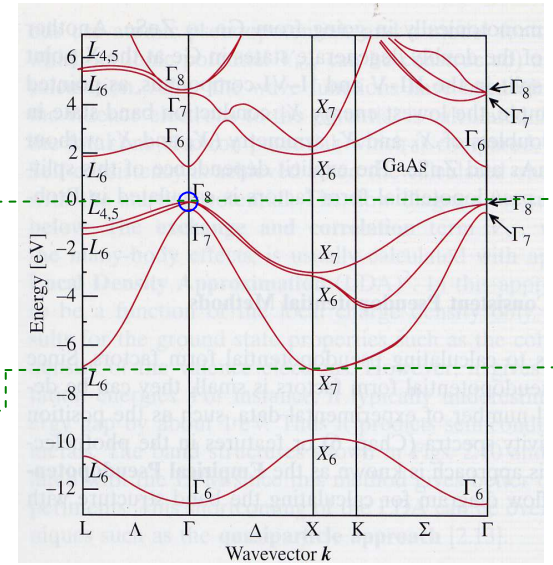


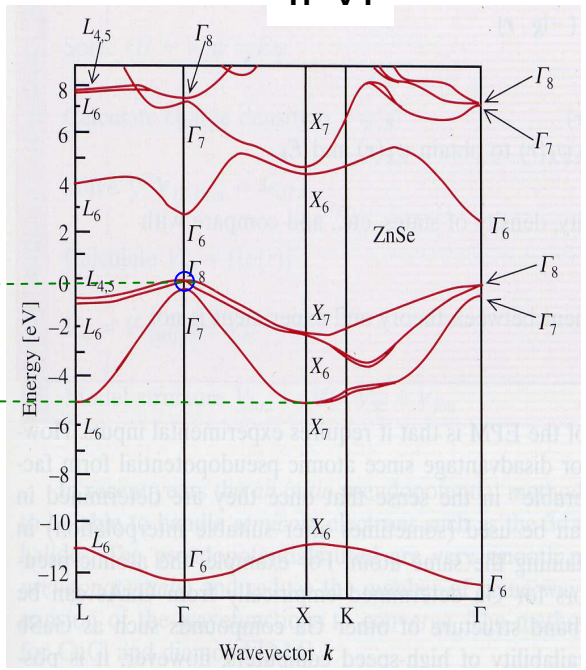
IV-IV

III-V

II-VI







indirect…….

direct…….

direct band gap

The band **gap energy** increases (increase of bonding strength)

The **width of the bands** shrinks, i.e. electrons more tightly bound!