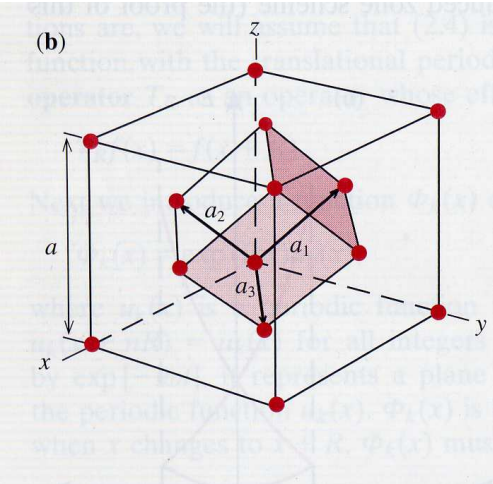
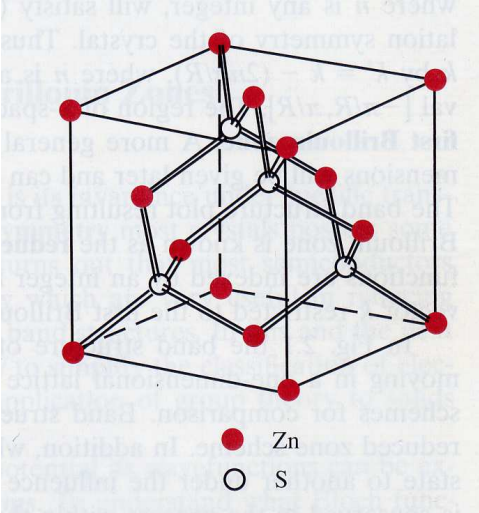
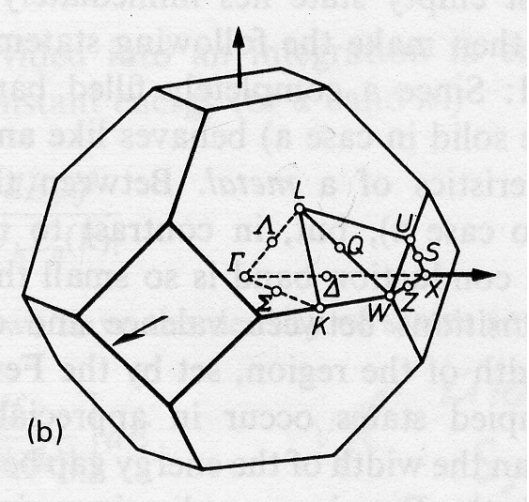
The Zincblende Lattice and BZ

…… valid for GaAs, ZnSe, InSb, …..







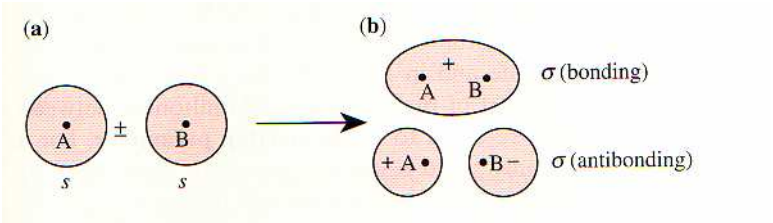
Lattice

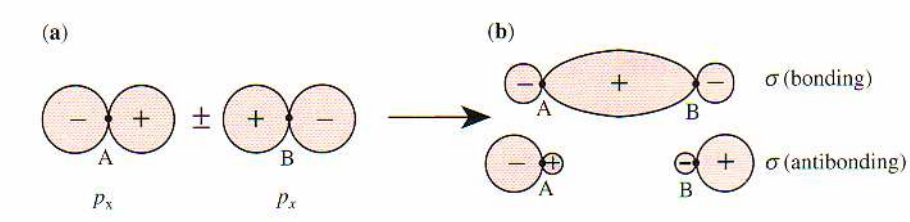
Basis of atoms

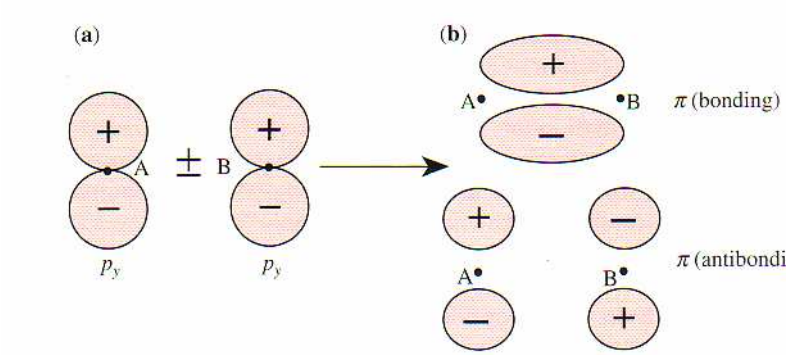
(1.) Brillouin zone

Band Structures by the LCAO Method

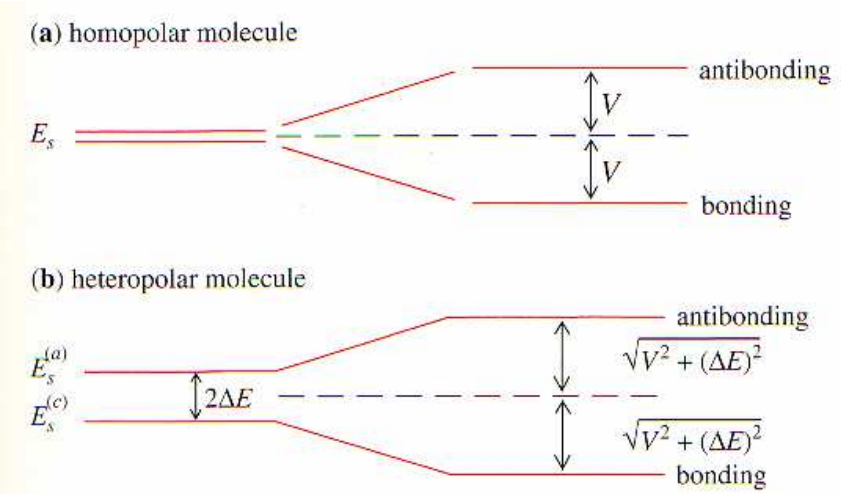
Starting point: bonds are formed from atomic orbitals.
Only s and p, and sometimes d orbitals are relevant for semiconductors





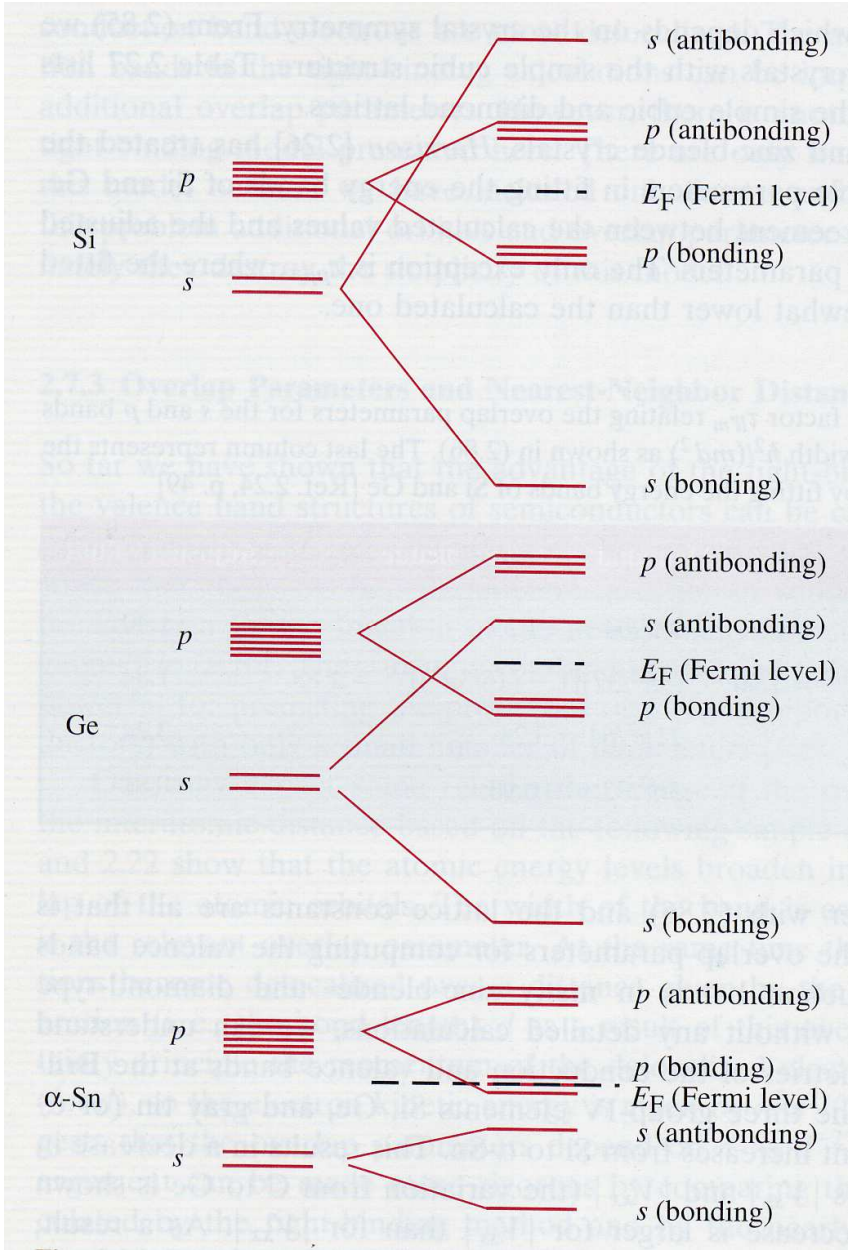


Atomic orbital energies split.



σ and π molecular orbitals are formed.

Band Structures by the LCAO Method

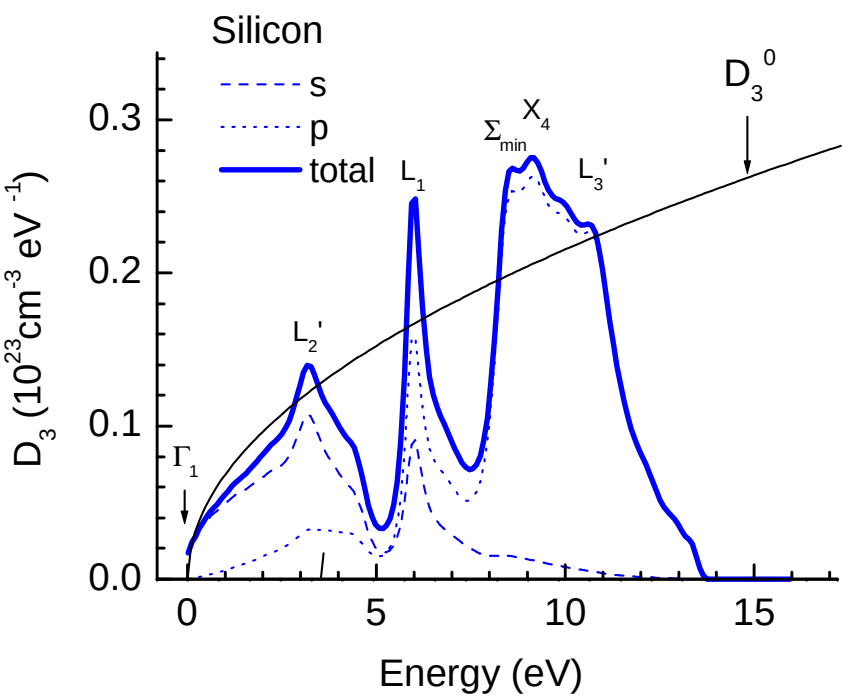


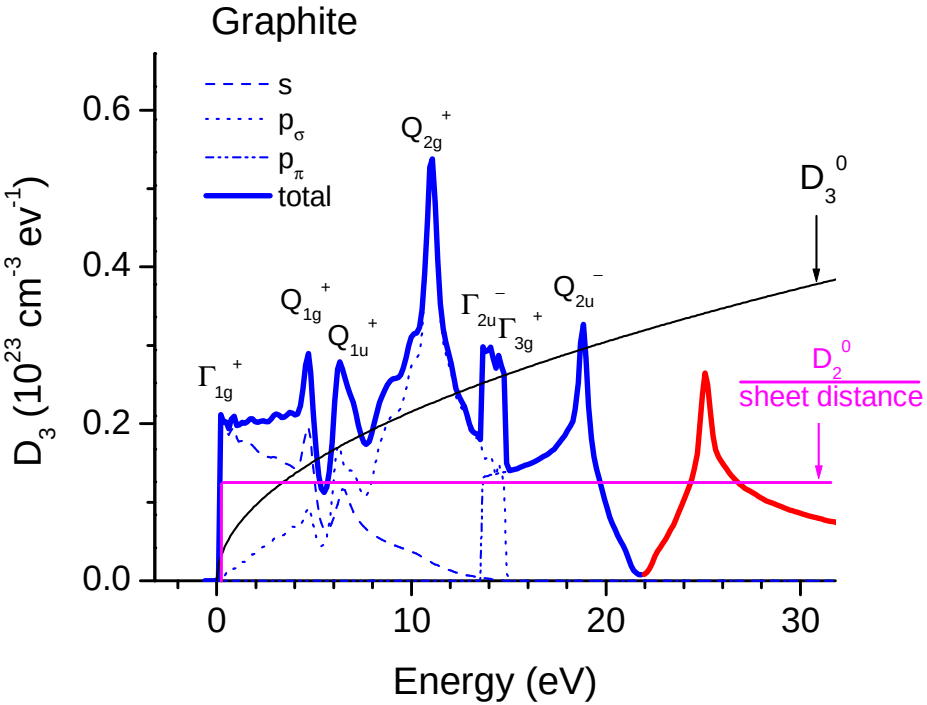
Split levels further broaden by nearest and next-nearest neighbour interaction and form

$\vec{k}$-dependent engergy bands in the BZ !

The Bloch waves keep (now $\vec{k}$-dependent) mixed atomic orbital characters, with reminescence to the atomic orbitals of the atoms!

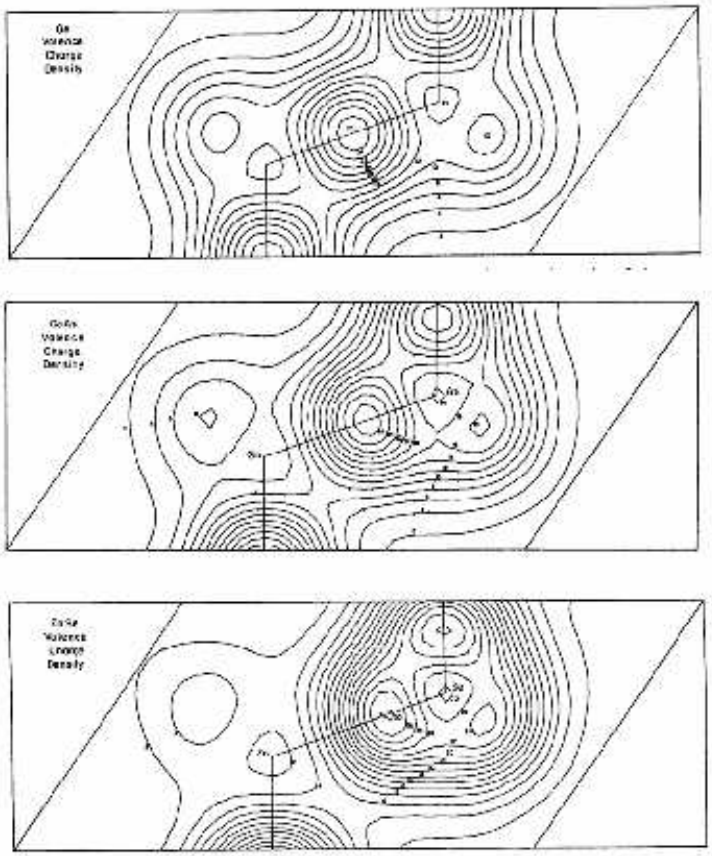
Partial DOS by the LCAO Method





- The LCAO approach yields automatically atomic orbital characters χ^ℓ for each Bloch wave!
- Otherwise, projection of the Bloch waves onto the Löwdin orbitals yields χ^ℓ as well!
- Weighting each Bloch wave by the χ^ℓ yields **partial densities** of states for the band structure of the solid

Valence Charge Density



Si

GaAs

ZnSe

Chelikowsky and Cohen

Contour plots of the valence charge density in Zincblende semiconductors

$$\rho(\vec{r}) = e\sum_{n=1}^{4}\sum_{\vec{k}\in B.Z.}\left|u_{n,\vec{k}}(\vec{r})\right|$$