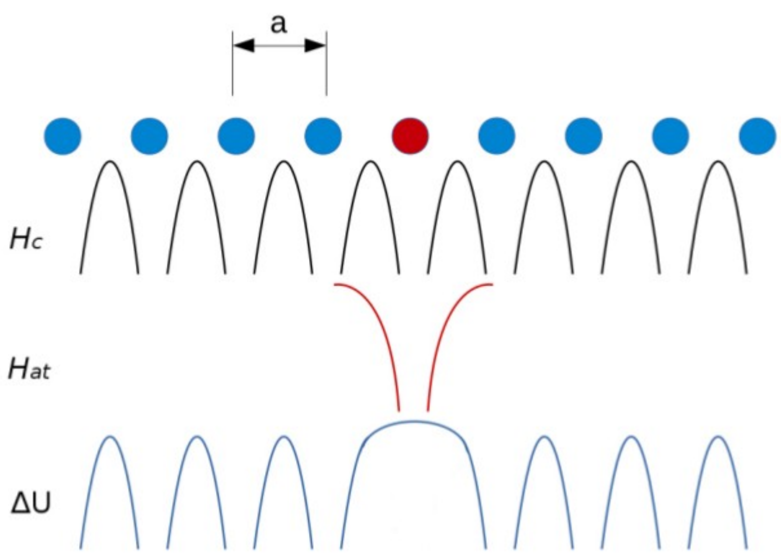
Tight Binding method for 1D atomic chain

- LCAO for a periodic atomic chain: the Tight Binding method
- s- and p-orbitals overlap integral: relation with band curvature
- overlap integral and bandwidth
- overlap integral and interatomic distance

Tight-Binding approximation



$$H_{at}(r)\phi_s(r) = \varepsilon_s \phi_s(r)$$

$$H_c \Psi = E\Psi,$$

$$\left(H_{at}(r) + \Delta U(r)\right)\Psi = E\Psi.$$

$$\Psi_k(r) = \sum_R \exp\left(ikR\right)\phi_s(r-R)$$

$$\begin{aligned} E(k) &= \varepsilon_s - \beta - 2\gamma(a)\cos(ka) \\ &\approx \varepsilon_s - \beta - 2\gamma(a)\left(1 - \frac{1}{2}(ka)^2\right) \\ &= \varepsilon_s - \beta - 2\gamma(a) + \gamma(a)(ka)^2 \end{aligned}$$

Comparison with “real” bandstructures

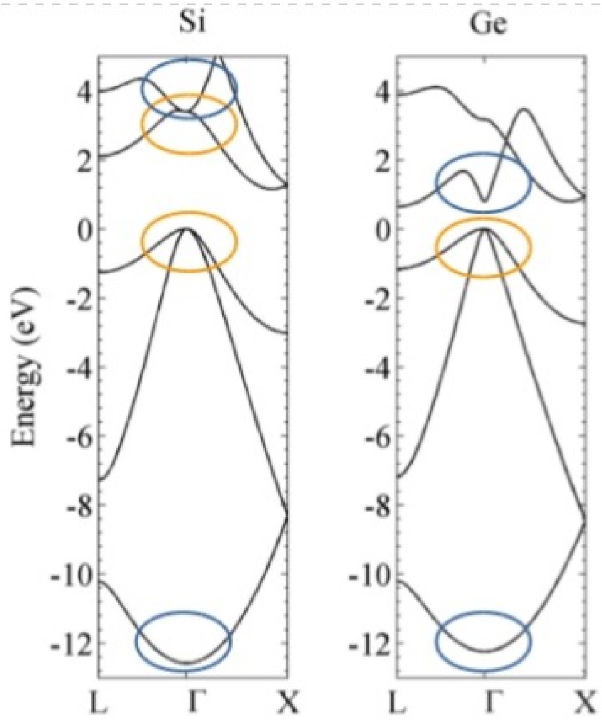


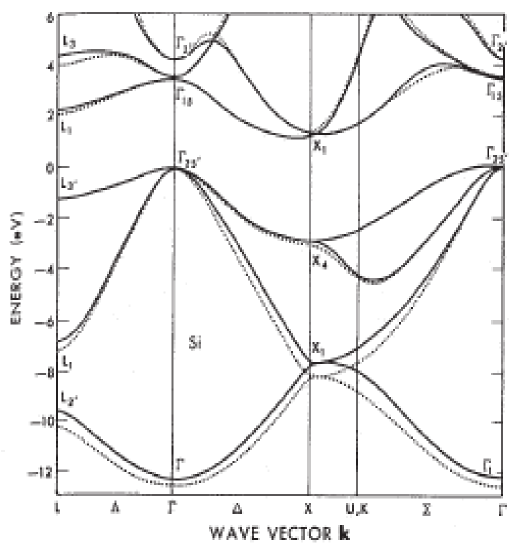
Figure 2.7: Bandstructure of Si and Ge taken from P. Moontragoon et al. J. Appl. Phys 112, 073106 (2012). The curvature of the bands around Γ (*i. e.* $k = 0$) are highlighted in blue (orange) for bands originating from s-type (p-type) orbitals.

Comparison with “real” bandstructures

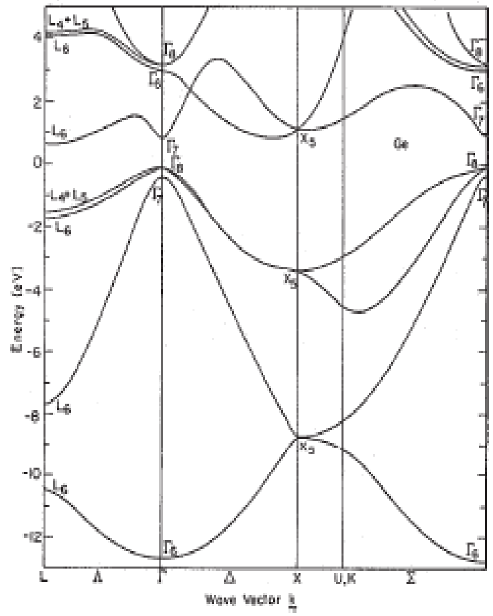
Relationship between the overlap integral γ and the energy width of the band

$$
\begin{aligned}
E(k) &= \varepsilon_s - \beta - 2\gamma(a)\cos(ka) \\
&\approx \varepsilon_s - \beta - 2\gamma(a)\left(1 - \frac{1}{2}(ka)^2\right) \\
&= \varepsilon_s - \beta - 2\gamma(a) + \gamma(a)(ka)^2
\end{aligned}
$$

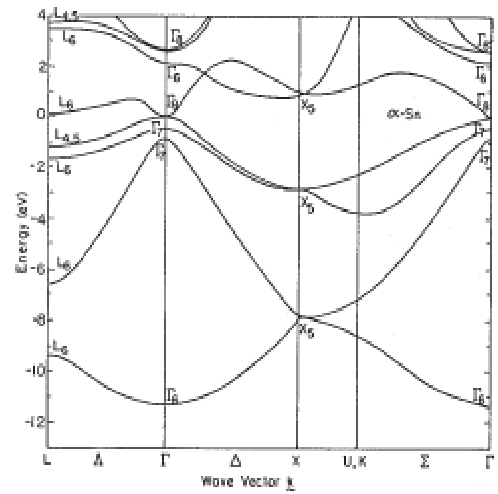
Si



Ge

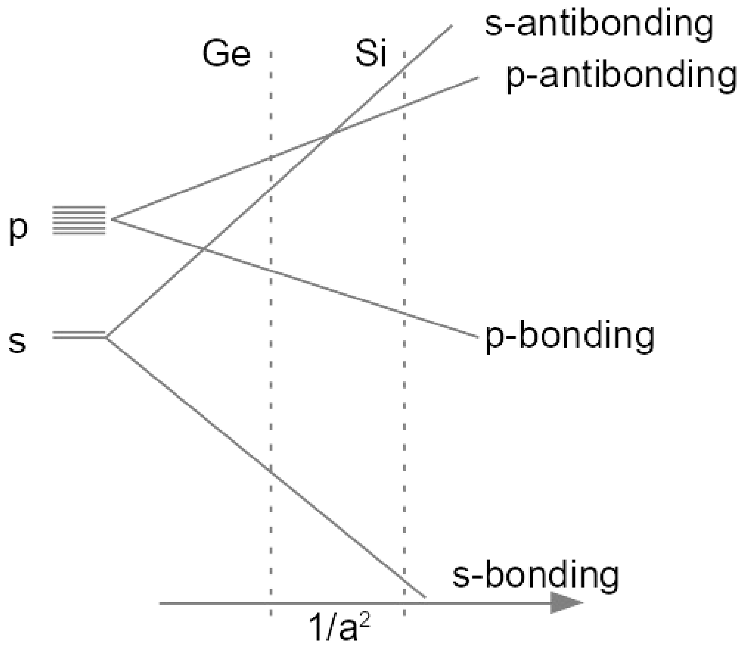


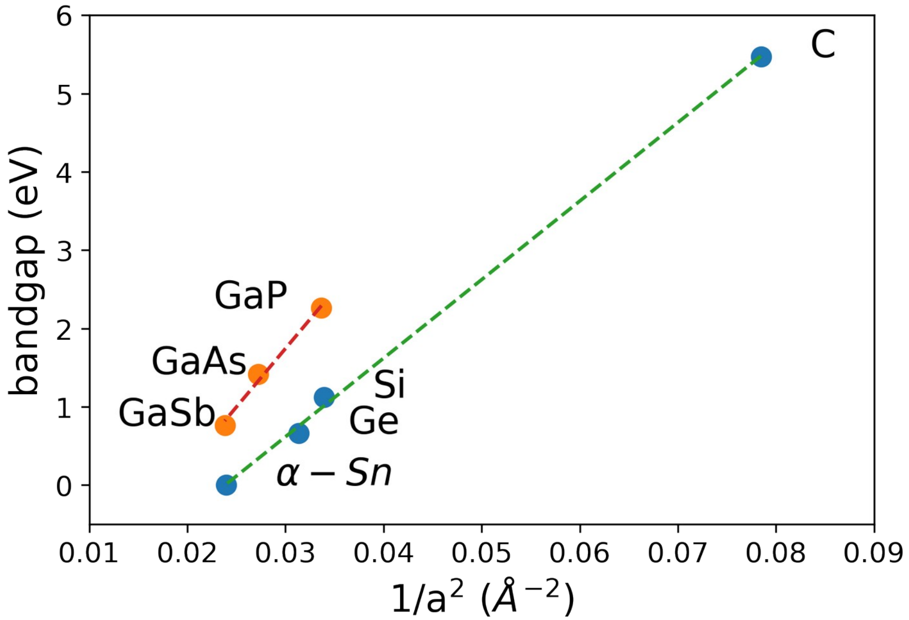
α-Sn



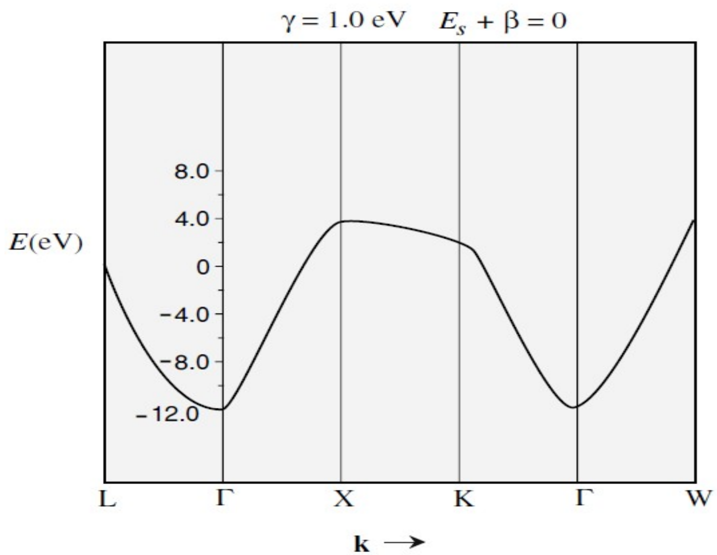
The dispersion around the Γ point (k≈0) of the Brillouin Zone can be described by means of the effective mass m*

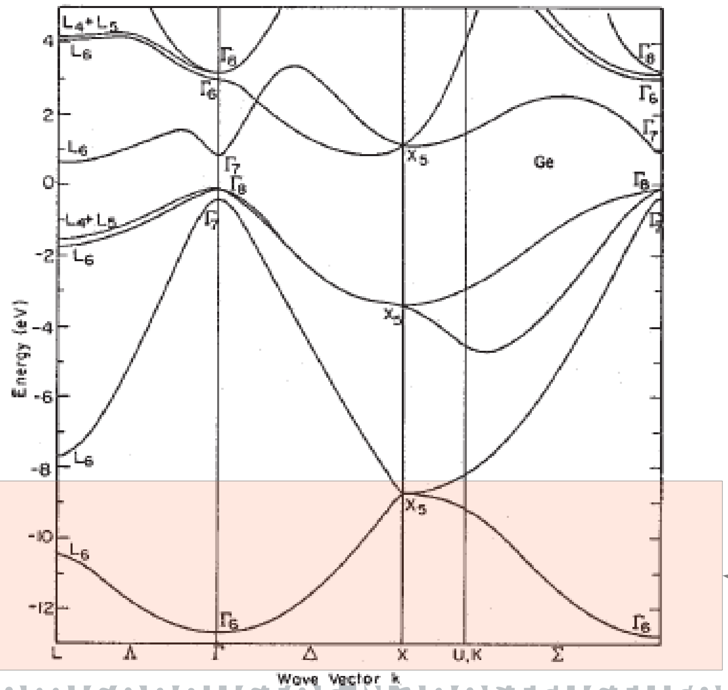
$$\gamma = \frac{\hbar^2}{2m^* a^2}. \qquad \gamma \propto \frac{1}{a^2}$$

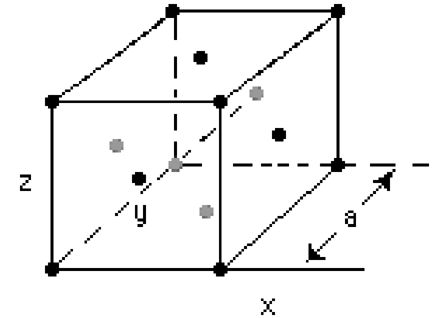




Comparison with “real” bandstructures







$$E(\mathbf{k}) = E_s - \beta_s - \sum_{\mathbf{R}} \gamma(\boldsymbol{R})\, e^{i\mathbf{k}\cdot\mathbf{R}}$$

For **R** spanning the first 12 near neighbours in a simple FCC lattice

$$\frac{a}{2}(\pm 1, \pm 1, 0);\ \frac{a}{2}(\pm 1, 0, \pm 1);\ \frac{a}{2}(0, \pm 1, \pm 1)$$

$$\begin{aligned} E(\mathbf{k}) \quad &= \quad E_s - \beta_s - \gamma \left[e^{i(k_x+k_y)a/2} + e^{i(k_x-k_y)a/2} \right. \\ &\qquad \left. + e^{i(-k_x+k_y)a/2} + e^{i(k_x-k_y)a/2} + \ldots \right] \\ &= \quad E_s - \beta_s - 4\gamma \left[\cos\frac{k_x a}{2} \cos\frac{k_y a}{2} \right. \\ &\qquad \left. + \cos\frac{k_y a}{2} \cos\frac{k_z a}{2} + \cos\frac{k_z a}{2} \cos\frac{k_x a}{2} \right] \end{aligned}$$

S-like bonding band