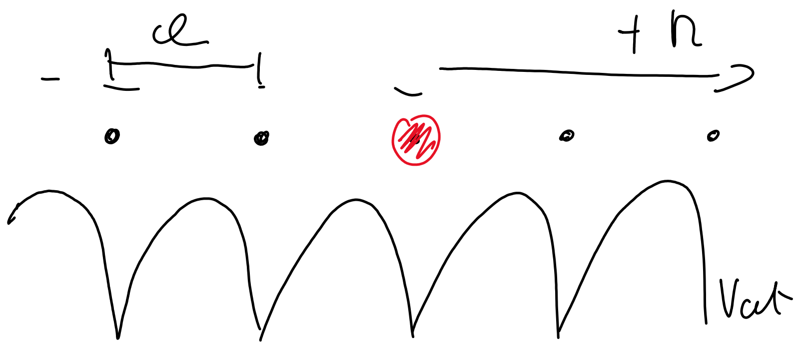
Tight Binding 1D

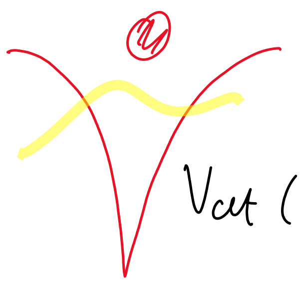
domenica 3 novembre 2024 21:38

Tight Binding method for 1D atomic chain

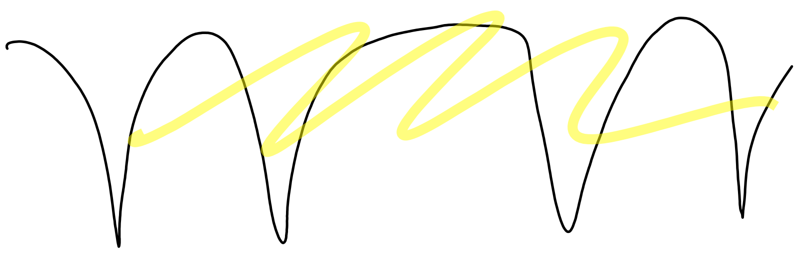
- LCAO for a periodic atomic chain: the Tight Binding method
- s- and p-orbitals overlap integral: relation with band curvature
- overlap integral and bandwidth
- overlap integral and interatomic distance



$$V_c = \sum_{R=-\infty}^{+\infty} V_{cel}$$



$V_{at}(r) \quad (r = \emptyset)$



$$\Delta U = \sum_{R \neq 0} V_{at}$$

$$H = T + V_{at}(r) + \Delta U \qquad \left(T + V_{at}(r)\right)\phi$$

V_c

R = LATTI

r = CONTI
VARIA

$$\psi = \sum_{R=-\infty}^{+\infty} e^{ik\underline{R}} \phi_s(r-R)$$

$$e^{ikr} u_k(r)$$

$$\boxed{\psi(r+R) = e^{ikR}\psi(r)}$$

$$\psi = \phi_s(r) + \sum_{R\neq 0} e^{ikR} \phi_s(r-R)$$

$$\left(T + V_{at}(r) + \Delta U\right)\left(\phi_s(r) + \sum_{R\neq 0} e^{ikR} \phi_s(r\right.$$

$$\shortparallel$$

$$E(k)\left(\phi_s(r) + \sum_{R\neq 0} e^{ikR} \phi_s(r-R\right.$$

$$\int \phi_s^*(r)\left(T + V_{at} + \Delta U\right)\left(\phi_s(r) + \sum_{R\neq 0} e^{ikR}\,\phi_s(r-R\right.$$

$$\shortparallel$$

$$\int \phi_s^*(r)\; E(k)\left(\phi_s(r) + \sum_{R\neq 0} e^{ikR}\,\phi_s(\right.$$

(1)

$$\int \phi_s^*\,(T+V_{at})\,\phi_s\,dr = \varepsilon \qquad (T+V_{\cdot}$$

(2)

$$\int \phi_s^*\,\Delta U\,\phi_s\,dr = -\beta$$

(3)

$$\int \phi_s^*\,(T+V_{at}) \sum_{R\neq 0} e^{ikR}\,\phi(r-R)\,dr = \sum_{R\neq 0}$$

$$= \sum_{R\neq 0} \int \phi_s^*(r-R)\,\underline{(T+V_{at})\,\phi_s(r)}\,d\cdot$$

$$= \underbrace{\sum_{R\neq 0} \varepsilon \int \phi_s^*(r-R)\,\phi_s(r)}_{\shortparallel\ \varnothing}$$

(4)

$$\int \phi_s(r)\;\Delta V \sum_{R\neq 0} e^{ikR}\,\phi_s(r-R)\,dr$$

$$\sum_{R\neq 0} e^{ikR} \int \phi_s(r)\, \Delta V\, \phi_s(r-R)\, dr = -\gamma(R)$$

$$\varepsilon - \beta - \sum_{R\neq 0} e^{ikR}\, \gamma(R) = E(k)$$

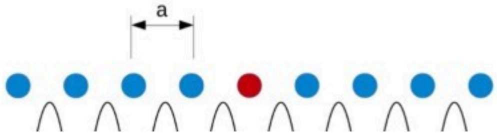
$$E(k) = \varepsilon - \beta - \sum_{R=0} e^{ikR}\, \gamma(R)$$

near neighbour interaction $R = \cdot$

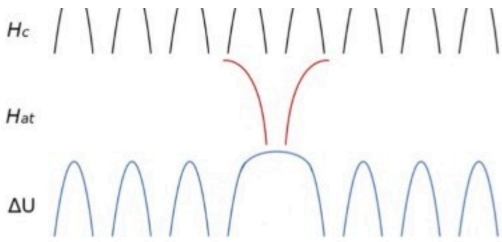
$$E(k) = \varepsilon - \beta - e^{ika}\gamma(a) - e^{-ika}\gamma$$

$$\underline{E(k) = \varepsilon - \beta - 2\gamma\cos(ka)}$$

Tight-Binding approximation



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



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

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

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

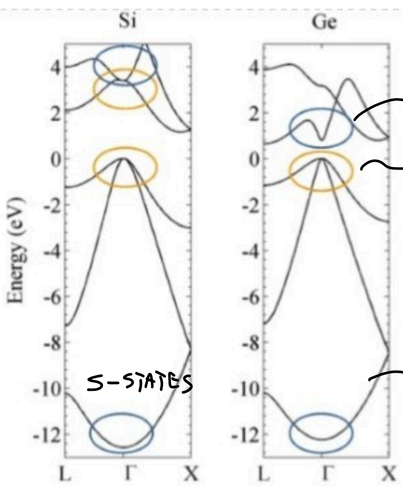
$ka \approx 0 \quad k \to \Gamma$

$\cos(ka) \approx 1 - \frac{1}{2}(ka)^2$

$\gamma > 0$ S-STATES

$\gamma < 0$ P-STATES

Comparison with “real” bandstructures



S-STATES

P-STATES

cos ka

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.

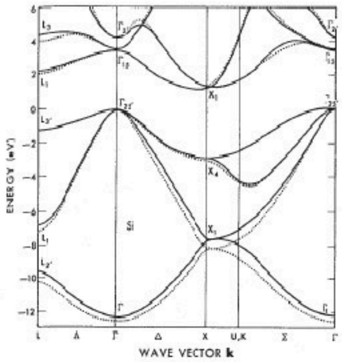
Comparison with “real” bandstructures

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

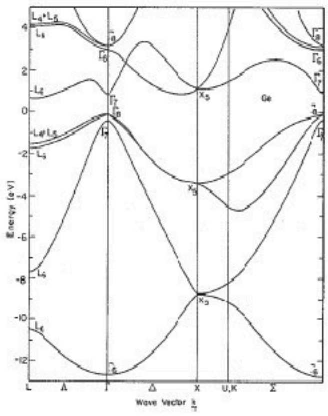
$$E(k) = \varepsilon_s - \beta - 2\gamma(a)\cos(ka)$$

$$\approx \varepsilon_s - \beta - 2\gamma(a)\left(1 - \frac{1}{2}(ka)^2\right)$$
$$= \varepsilon_s - \beta - 2\gamma(a) + \gamma(a)(ka)^2$$

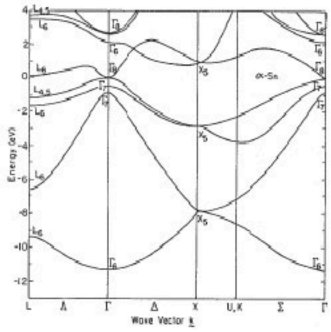
Si



Ge



α-Sn



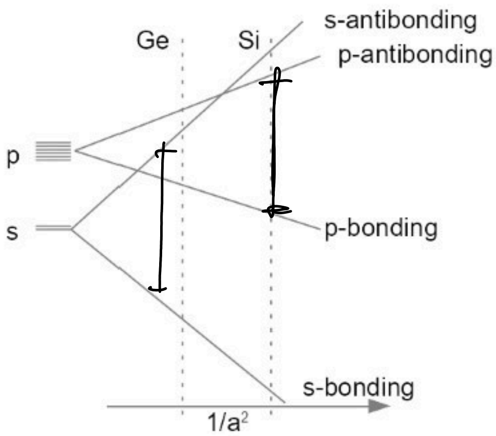
Overlap integral and effective mass

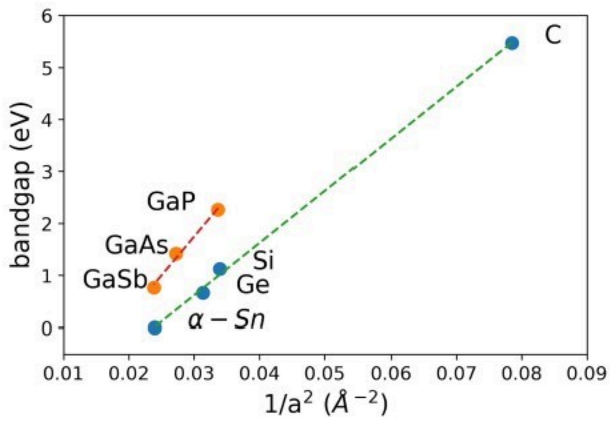
The dispersion around the Γ point (k≈0) of the Brillouin Zone can be described by means of the effective mass m*

$\int$ $k=0$

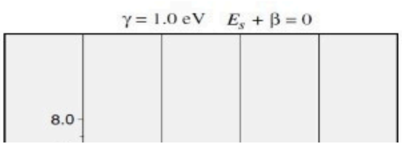
$$\gamma = \frac{\hbar^2}{2m^* a^2}. \qquad \gamma \propto \frac{1}{a^2}$$

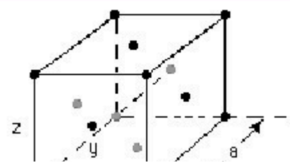
$E(k)$ $\quad \gamma k^2 a^2 = \frac{\hbar^2 k^2}{2m^*}$



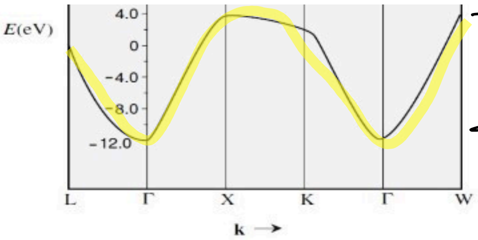


Comparison with “real” bandstructures

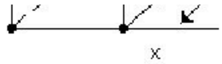




FC



2γ

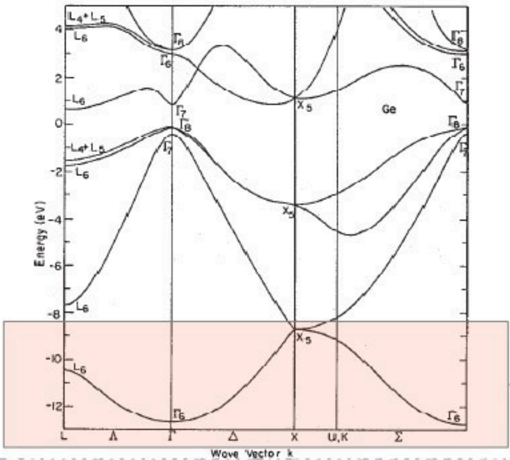


$$E(\mathbf{k}) = E_s - \beta_s - \sum_{\mathbf{R}} \gamma(\boldsymbol{R})\, e^{i\mathbf{k}\cdot\mathbf{R}}$$

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

$$\frac{a}{2}(\pm1,\pm1,0);\ \frac{a}{2}(\pm1,0,\pm1);\ \frac{a}{2}(0,\pm1,\pm1)$$

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



S-like bonding band