# The k-dot-p method

- The k-dot-p Hamiltonian $\vec{k}\cdot\vec{p}$
- A two-band simplified model: electron effective mass and bandgap
- Bandgap and electron effective mass
- The eight-band k-dot-p Hamiltonian



$$(T+V)\,u_{m,k}(r)\,e^{ikr} = E_m(k)\,e^{ikr}$$

$$T = -\frac{\hbar^2\nabla^2}{2m_0} \qquad -\hbar^2\nabla^2\psi = -i\hbar\vec{\nabla}\cdot\left(-i\hbar\vec{\nabla}\psi\right)$$

$p$

$$T = \frac{p^2}{2m_0} \rightarrow \frac{(m_0 v)^2}{2m_0} = \frac{1}{2}m_0 v^2$$

$$-i\hbar\vec{\nabla}\cdot\left(u\,e^{i\vec{k}\vec{r}}\right) = \left(\hbar\vec{k}\,e^{ikr}\,u(r) - i\hbar\right.$$

$$-i\hbar\vec{\nabla}\cdot\left(\sim\right) = -i\hbar$$

$$\frac{1}{2m_0}\left(\hbar^2 k^2 u(r)\, \cancel{e^{i\vec{k}\vec{r}}} + \left(2\hbar\, \vec{k}\cdot\vec{\nabla} u\right) \cancel{e^{i\vec{k}\vec{r}}} - (\right.$$

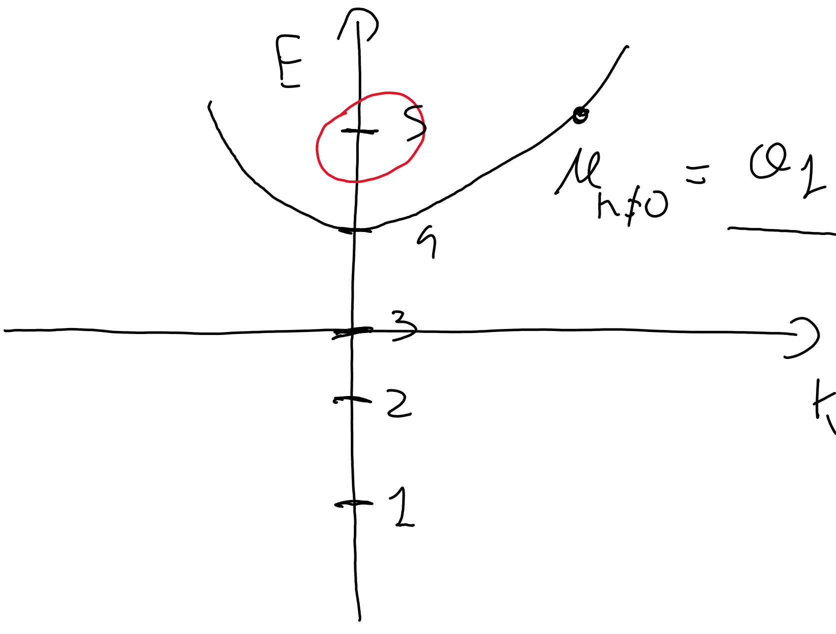
$$-\frac{\hbar^2\nabla^2}{2m_0}\, u_{m,k}(r) + \frac{\hbar}{m_0}\,\vec{k}\cdot\vec{p}\; u_{m,k}(r) + \frac{\hbar^2 k^2}{2m_0}\, u_{m,k}(r) + |$$

$$\left(\underline{-\frac{\hbar^2\nabla^2}{2m_0}u + Vu} + \underbrace{\frac{\hbar}{m_0}\,\vec{k}\cdot\vec{p}\,u + \frac{\hbar^2k^2}{2m_0}u}_{k\ ,\ k^2}\right) = E\, u$$

Perturbation THEORY

$k = 0$

$$\left(-\frac{\hbar^2\nabla^2}{2m_0}\, u_{k=0} + V u_{k=0}\right) = E_n(k=0)\, u_{k=0}$$




$$u_{k\neq 0} = a_1 u_1 + a_2 u_2 + a_3$$

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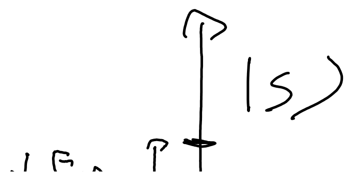



$$\left(-\frac{\hbar^2\nabla^2}{2m_0} + V\right)|s\rangle = \frac{E_0}{2}\; |$$

$$\frac{+E_g}{2}$$

$$\frac{-E_g}{2} \quad |P\rangle \longrightarrow \left(-\frac{\hbar^2 p^2}{2m_0} + V\right)|P\rangle = -\frac{E_g}{2}$$

$$\boxed{\overset{H}{\left(-\frac{\hbar^2 p^2}{2m_0} + V + \frac{\hbar}{m_0}\vec{k}\cdot\vec{p} + \frac{\hbar^2 k^2}{2m_0}\right)}}\,\phi = E$$

$$\phi = a_s|s\rangle + a_p|P\rangle$$

$$\begin{array}{c|cc} & |s\rangle & |P\rangle \\ \hline \langle s| & \frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_0} & \frac{\hbar}{m_0} k P_{cv} \\ \langle P| & \frac{\hbar}{m_0} k P_{cv} & -\frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_0} \end{array} \quad E(k)$$

$$H_{11} = \langle s| -\frac{\hbar^2 p^2}{2m_0} + V + \frac{\hbar}{m_0}\vec{k}\cdot\vec{p} + \frac{\hbar^2 k^2}{2m_0} |s\rangle$$

$$= \frac{E_g}{2} + \frac{\hbar}{m_0}\vec{k}\cdot\underset{\emptyset}{\underset{\parallel}{\langle s|\vec{p}|s\rangle}} + \frac{\hbar^2 k^2}{2m_0}\langle s$$

$$H_{12} = \langle s| -\frac{\hbar^2 p^2}{2m_0} + V + \frac{\hbar \vec{k}\cdot\vec{p}}{m_0} + \frac{\hbar^2 k^2}{2m_0} |P\rangle$$

$$= -\frac{E_g}{2}\underset{\substack{\| \\ \emptyset}}{\langle S|P\rangle} + \frac{\hbar^2 k^2}{2m_0}\underset{\substack{\| \\ \emptyset}}{\langle S|P\rangle} + \frac{\hbar}{m_0}\vec{k}\cdot$$

$$= \frac{\hbar}{m_0}\vec{k}\cdot\vec{P}_{cv}$$

## The k-dot-p method

By substituting the Bloch wavefunction $u_k(\mathbf{r})exp\,(i\mathbf{k}\cdot\mathbf{r})$

in the crystal Schrödinger equation $\left(\frac{\mathbf{p}^2}{2m_0}+V(\mathbf{r})\right)u_k(\mathbf{r})exp\,(i\mathbf{k}\cdot\mathbf{r}) = E(\mathbf{k})u_k(\mathbf{r})exp\,(i\mathbf{k}\cdot\mathbf{r})$

where $\mathbf{p} = -i\hbar\nabla$ is the momentum operator

we obtain an equation for the periodic part of the wavefunction

$$\left(\frac{\mathbf{p}^2}{2m_0}+V(\mathbf{r})+\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}+\frac{\hbar^2k^2}{2m_0}\right)u_k(\mathbf{r}) = E(\mathbf{k})u_k(\mathbf{r}).$$

In this equation the k-dot-p and k² terms can be treated as a perturbation and the solutions are obtained as a linear combination of the "unperturbed" eigenstates

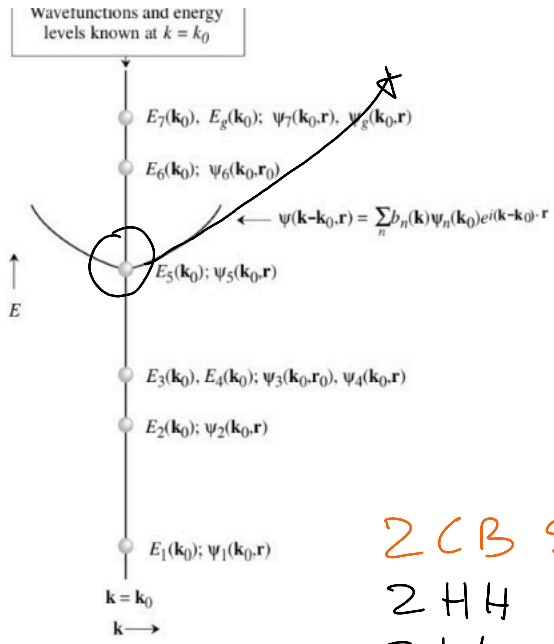
$$\left(\frac{\mathbf{p}^2}{2m_0}+V(\mathbf{r})\right)u_0(\mathbf{r}) = E(\mathbf{k}=0)u_0(\mathbf{r})$$

This can be done in two ways: (1) using perturbation theory

(2) using a matrix representation and a finite base set



## The k-dot-p method




2CB Si
2HH
2LH
2SO

In k-dot-p the band dispersion around a symmetry point $k_0$ is obtained as a linear combination of $k=k_0$ (orthogonal) states.

The larger the number of states the larger the fraction of the Brilloiun zone that can be mapped.

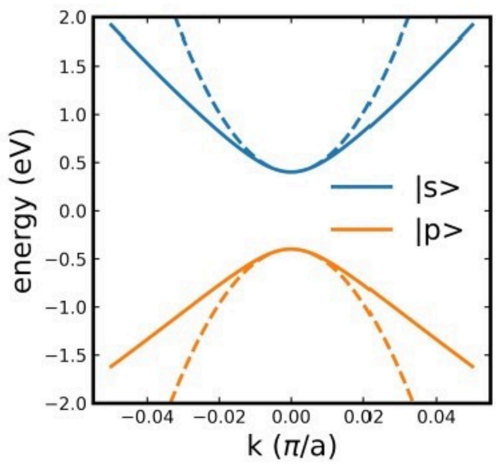
K-dot-p methods are labelled by the number of states (including spin degeneracy) which are used as a base

We talk about
6-bands, 8-bands, 30-bands k-dot-p



## The k-dot-p method: use of a limited base set

$$\left(\frac{p^2}{2m_0} + V(r) + \frac{\hbar}{m_0}k\cdot p + \frac{\hbar^2k^2}{2m_0}\right)(a_s|s> + a_p|p>) = E(k)\,(a_s|s> + a_p|p>)$$



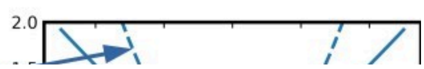

$$det\begin{vmatrix} E_g/2 + \frac{\hbar^2k^2}{2m_0} - E(k) & \frac{\hbar}{m_0}kp_{cv} \\ \frac{\hbar}{m_0}kp^*_{cv} & -E_g/2 + \frac{\hbar^2k^2}{2m_0} - E(k) \end{vmatrix} = 0$$

$$\begin{aligned} E(k) &= \frac{\hbar^2k^2}{2m_0} \pm \frac{E_g}{2}\sqrt{1 + \frac{4\hbar^2k^2}{m_0}\frac{p^2_{cv}}{E^2_g}} \\ &= \frac{\hbar^2k^2}{2m_0} \pm \frac{E_g}{2}\sqrt{1 + \frac{2\hbar^2k^2}{m_0}\frac{E_p}{E^2_g}}, \end{aligned}$$

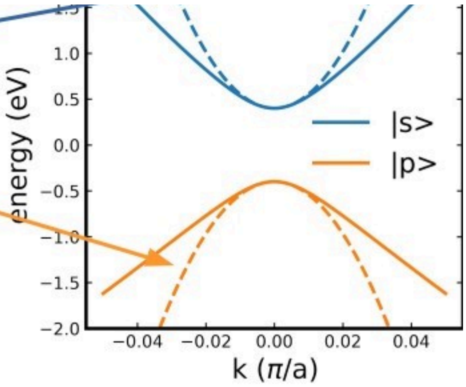
$$E_p = 2p^2_{cv}/m_0$$



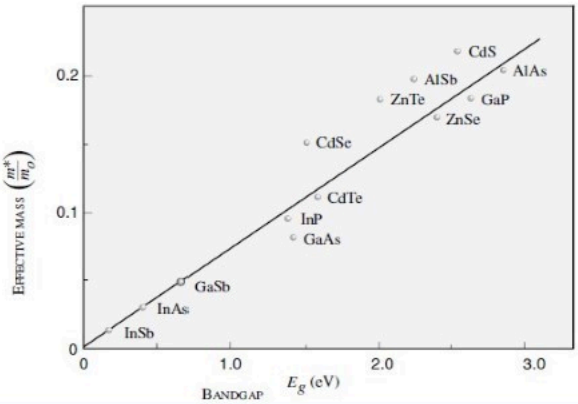
## The k-dot-p method: use of a limited base set



$$E(k) = \begin{cases} \frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_0}\left(1 + \frac{E_p}{E_g}\right) \approx \frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_0}\frac{E_p}{E_g} \\ -\frac{E_g}{2} + \frac{\hbar^2 k^2}{2m_0}\left(1 - \frac{E_p}{E_g}\right) \approx -\frac{E_g}{2} - \frac{\hbar^2 k^2}{2m_0}\frac{E_p}{E_g} \end{cases}$$



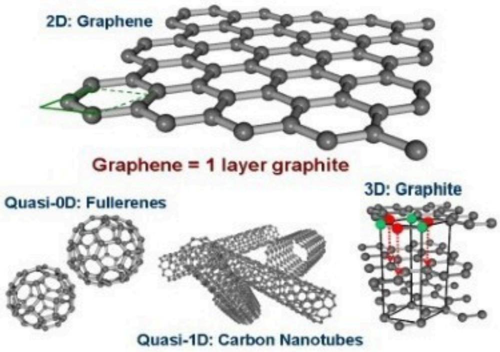

$$m^* \approx m_0 \frac{E_g}{E_p}.$$

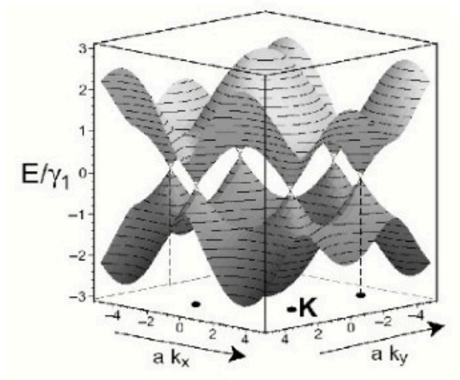





## Effective mass in a zero gap semiconductor

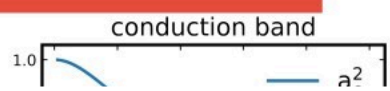
In graphene, there are six degenerate couples of CB minima/VB maxima.
The bandgap is approaching zero resulting in a zero effective mass!






## Band mixing

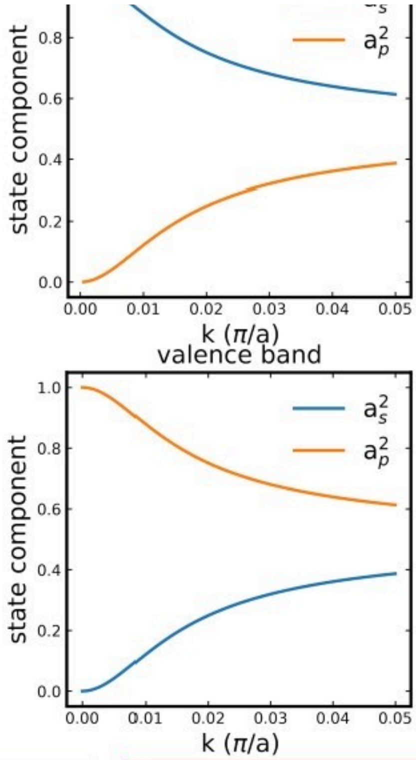


$$\Psi = (a_s|s> + a_p|p>)$$

$$\begin{bmatrix} E_g/2 + \frac{\hbar^2 k^2}{2m_0} - E(k) & \frac{\hbar}{m_0} k p_{cv} \\ \frac{\hbar}{m_0} k p_{cv}^* & -E_g/2 + \frac{\hbar^2 k^2}{2m_0} - E(k) \end{bmatrix} \begin{bmatrix} a_s \\ a_p \end{bmatrix} = 0$$

$$a_s(k) = \frac{\left(E_g/2 + \frac{\hbar^2 k^2}{2m_0} - E(k)\right)\left(-E_g/2 + \frac{\hbar^2 k^2}{2m_0} - E(k)\right)}{\left(\frac{\hbar}{m_0} k p_{cv}\right)^2}$$

$$a_p(k) = \frac{\left(\left(\frac{\hbar^2 k^2}{2m_0} - E(k)\right)^2 - E_g^2/4\right)\left(E_g/2 + \frac{\hbar^2 k^2}{2m_0} - E(k)\right)}{\left(\frac{\hbar}{m_0} k p_{cv}\right)^3}$$






## The k-dot-p method: eight bands with spin-orbit interaction

The k-dot-p method can be extended to treat spin-orbit interaction in the VB

$$Hu_{n\mathbf{k}}(\mathbf{r}) = \left(H_0 + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar}{4m_0^2c^2}\nabla V \times \mathbf{p}\cdot\boldsymbol{\sigma}\right)u_{n\mathbf{k}}(\mathbf{r}) = E' u_{n\mathbf{k}}(\mathbf{r})$$

Spin-orbit term Pauli matrix

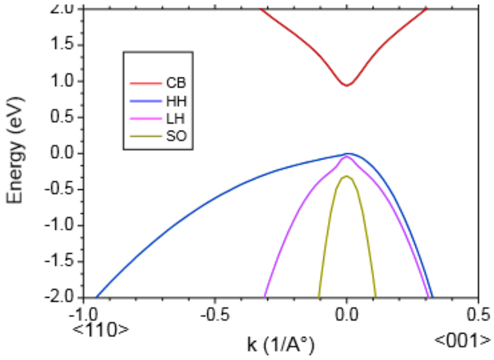
In this case we can use the "total angular momentum" states + 2 s-like CB states for the expansions.

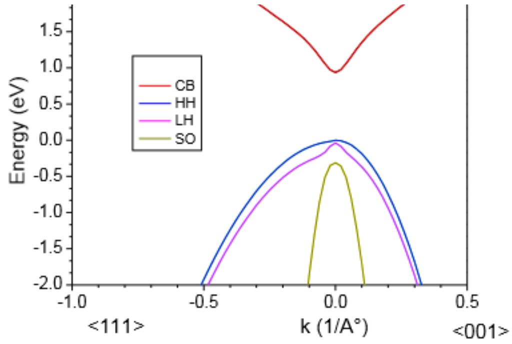
Some numerical solutions using such 8 band k-dot-p scheme are shown in the next two slides.

| | $\lvert iS\uparrow\rangle$ | $\lvert\frac{3}{2},\frac{1}{2}\rangle$ | $\lvert\frac{3}{2},\frac{3}{2}\rangle$ | $\lvert\frac{1}{2},\frac{1}{2}\rangle$ | $\lvert iS\downarrow\rangle$ | $\lvert\frac{3}{2},-\frac{1}{2}\rangle$ | $\lvert\frac{3}{2},-\frac{3}{2}\rangle$ | $\lvert\frac{1}{2},-\frac{1}{2}\rangle$ |
|---|---|---|---|---|---|---|---|---|
| $\langle iS\uparrow\rvert$ | $\frac{\hbar^2k^2}{2m_0}$ | $-\sqrt{\frac{2}{3}}P\hbar k_z$ | $P\hbar k_+$ | $\frac{1}{\sqrt{3}}P\hbar k_z$ | 0 | $-\frac{1}{\sqrt{3}}P\hbar k_-$ | 0 | $-\sqrt{\frac{2}{3}}P\hbar k_-$ |
| $\langle\frac{3}{2},\frac{1}{2}\rvert$ | $-\sqrt{\frac{2}{3}}P\hbar k_z$ | $-\varepsilon_0+\frac{\hbar^2k^2}{2m_0}$ | 0 | 0 | $\frac{P}{\sqrt{3}}\hbar k_-$ | 0 | 0 | 0 |
| $\langle\frac{3}{2},\frac{3}{2}\rvert$ | $P\hbar k_-$ | 0 | $-\varepsilon_0+\frac{\hbar^2k^2}{2m_0}$ | 0 | 0 | 0 | 0 | 0 |
| $\langle\frac{1}{2},\frac{1}{2}\rvert$ | $\frac{1}{\sqrt{3}}P\hbar k_z$ | 0 | 0 | $-\varepsilon_0-\Delta+\frac{\hbar^2k^2}{2m_0}$ | $\sqrt{\frac{2}{3}}P\hbar k_-$ | 0 | 0 | 0 |
| $\langle iS\downarrow\rvert$ | 0 | $\frac{P}{\sqrt{3}}\hbar k_+$ | 0 | $\sqrt{\frac{2}{3}}P\hbar k_+$ | $\frac{\hbar^2k^2}{2m_0}$ | $-\sqrt{\frac{2}{3}}P\hbar k_z$ | $P\hbar k_-$ | $\frac{1}{\sqrt{3}}P\hbar k_z$ |
| $\langle\frac{3}{2},-\frac{1}{2}\rvert$ | $-\frac{1}{\sqrt{3}}P\hbar k_+$ | 0 | 0 | 0 | $-\sqrt{\frac{2}{3}}P\hbar k_z$ | $-\varepsilon_0+\frac{\hbar^2k^2}{2m_0}$ | 0 | 0 |
| $\langle\frac{3}{2},-\frac{3}{2}\rvert$ | 0 | 0 | 0 | 0 | $P\hbar k_+$ | 0 | $-\varepsilon_0+\frac{\hbar^2k^2}{2m_0}$ | 0 |
| $\langle\frac{1}{2},-\frac{1}{2}\rvert$ | $-\sqrt{\frac{2}{3}}P\hbar k_+$ | 0 | 0 | 0 | $\frac{P}{\sqrt{3}}\hbar k_z$ | 0 | 0 | $-\varepsilon_0-\Delta+\frac{\hbar^2k^2}{2m_0}$ |

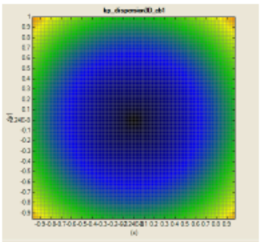


## Eight bands k-dot-p: Ge bandstructure

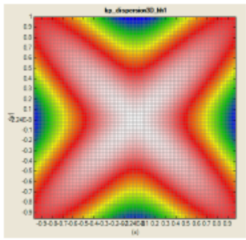


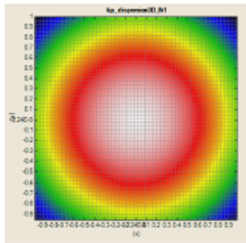

CB



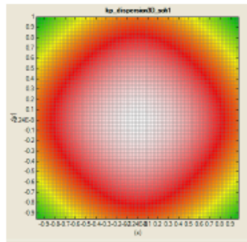
HH



LH

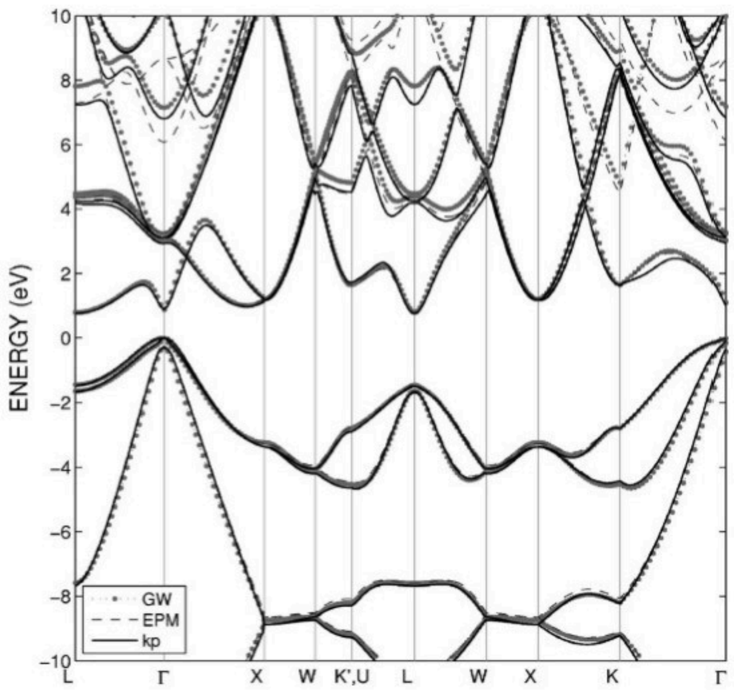


SO





# 30 bands k-dot-p: Ge bandstructure




D. Rideau, M. Feraille, L. Ciampolini, M. Minondo, C. Tavernier, H. Jaouen, and A. Ghetti, Phys. Rev. B 74, 1 (2006).