Electronic properties of solids - Tight-binding and Band Theory

Lecture 15

CHM 637
Chemistry & Physics of Materials

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Lecture Plan

- Simple motivation to the tight-binding approach
- Energy bands, Brillouin zones and band-structure
- Typical semiconductors and insulators

General Approach for Bands in Solids

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})$$ — Bloch theorem

$$u_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r}+\vec{R})$$ — $\vec{R} \rightarrow$ lattice vector

$$v_{cry}(\vec{r}+\vec{R}) = v_{cry}(\vec{r})$$

$$\hat{H} = -\frac{\nabla^2}{2} + v_{cry}(\vec{r})$$

$$\left[\hat{T}_a, \hat{H}\right] = 0$$

$$\hat{H}\,\psi_{n\vec{k}}(\vec{r}) = \varepsilon_n(\vec{k})\,\psi_{n\vec{k}}(\vec{r})$$

n ↓ Band index

$\vec{k}$ → crystal momentum (quantum no.s emerging from translational symmetry)

$$\left\{-\frac{\nabla^2}{2} + V_{cry}(\vec{r})\right\}\left(e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})\right) = \varepsilon_n(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})$$

$$\nabla^2\left(e^{i\vec{k}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r})\right) = e^{i\vec{k}\cdot\vec{r}}\left(\vec{\nabla}+i\vec{k}\right)^2 u_{n\vec{k}}(\vec{r})$$

$\nabla^2 \rightarrow \vec{\nabla}\cdot\vec{\nabla}$

$$\Rightarrow \boxed{\left\{-\frac{\left(\vec{\nabla}+i\vec{k}\right)^2}{2} + V_{cry}(\vec{r})\right\} u_{n\vec{k}}(\vec{r}) = \varepsilon_n(\vec{k})\, u_{n\vec{k}}(\vec{r})}$$

$$V_{cry}(\vec{r}) = \sum_{\vec{G}} V_{cry}(\vec{G})\, e^{i\vec{G}\cdot\vec{r}}$$

Lattice Fourier Series

$\vec{G} \rightarrow$ Reciprocal Lattice vector.

$$= \sum_{l}\sum_{m}\sum_{n} V_{cry}(l,m,n)\, e^{-i\frac{2\pi}{a}(lx+my+nz)}$$

(for a cubic lattice)

$$V_{cry}(\vec{G}) = \frac{1}{\Omega}\int_{\Omega} d^3r\, e^{-i\vec{G}\cdot\vec{r}}\, V_{cry}(\vec{r})$$

$$\boxed{U_{n\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{n\vec{k}}(\vec{G})\, e^{i\vec{G}\cdot\vec{r}}}$$

$$\Rightarrow \sum_{\vec{G}'} \left\{ \frac{(\vec{k}+\vec{G})^2}{2} \delta_{\vec{G},\vec{G}'} + V_{cry}(\vec{G}-\vec{G}') \right\} C_{n\vec{k}}(\vec{G}')$$

$$= \varepsilon_n(\vec{k})\, C_{n\vec{k}}(\vec{G})$$

Solve by choosing a cutoff $|\vec{G}|$

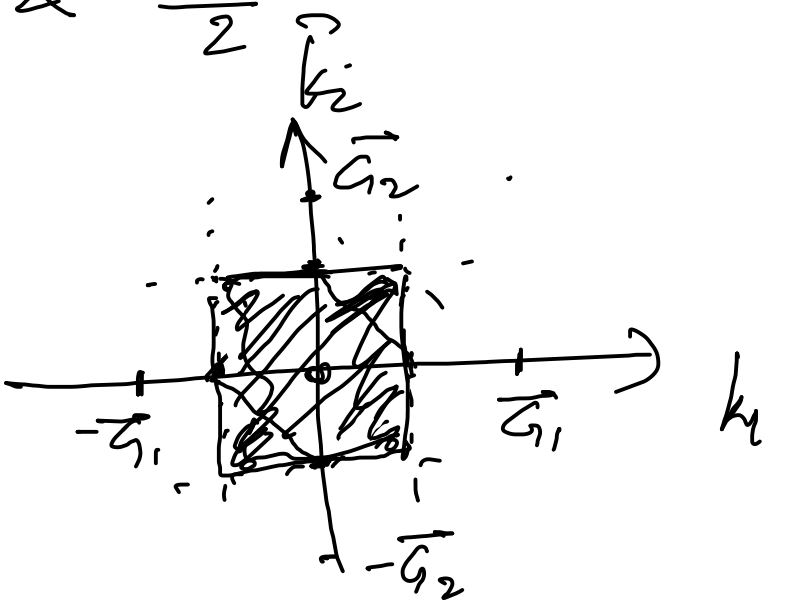
$$\Longrightarrow \left\{ \varepsilon_n(\vec{k}),\ u_{n\vec{k}}(\vec{r}) \right\} \Rightarrow \text{Band structure}$$

$$V_{cry}(\vec{r}) = \sum_{\vec{R}} \sum_{\mu} v^{ion}(\vec{r} - \vec{u}_\mu - \vec{R})$$

First Brillouin zone:

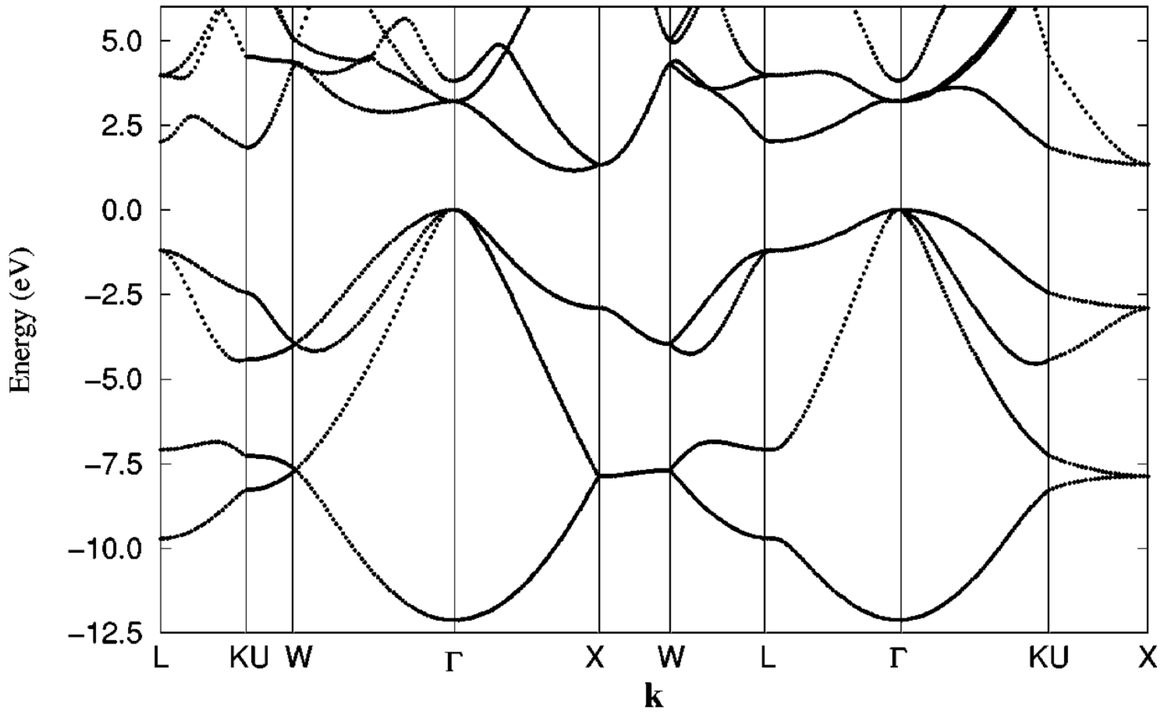
$$\vec{k} = f_1 \vec{G}_1 + f_2 \vec{G}_2 + f_3 \vec{G}_3$$

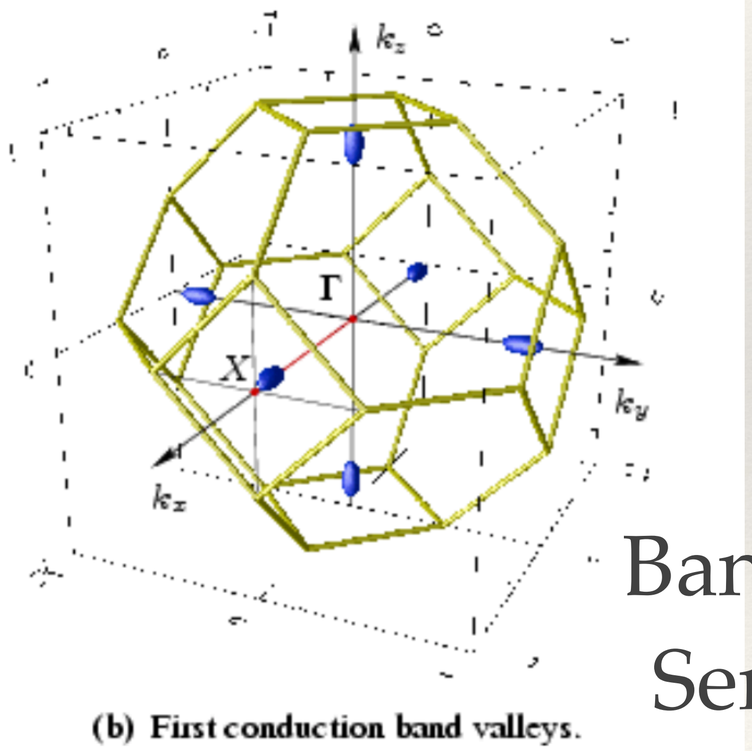
where f_1, f_2, f_3 are real numbers between $-\frac{|\vec{G}_i|}{2}$ & $\frac{|\vec{G}_i|}{2}$



Typical band structures

Silicon crystal





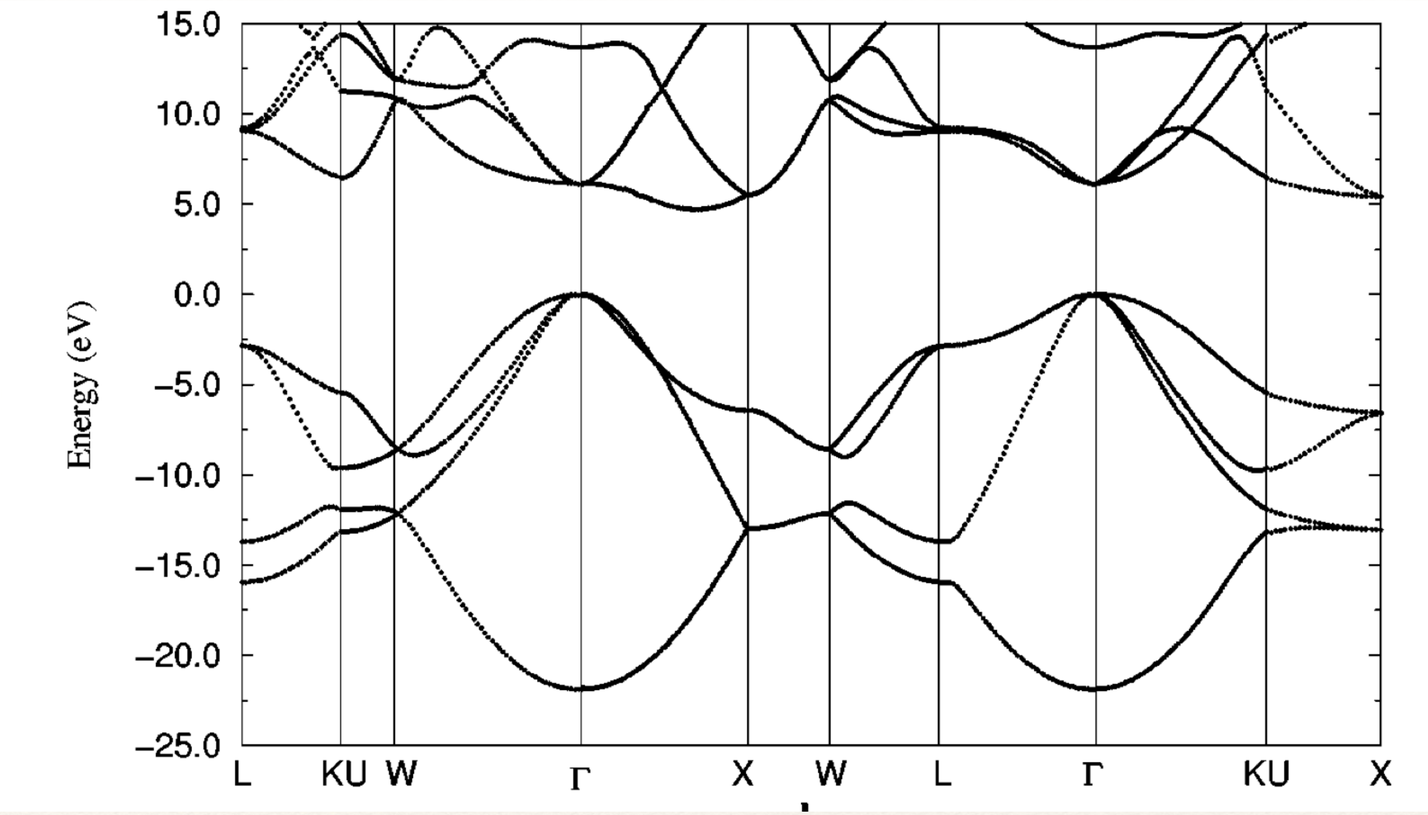
(b) First conduction band valleys.

Band-gap ~ 1 eV
Semiconductor

Source: PRB **59**, 5536 (1999)

Typical band structures

C (Diamond)

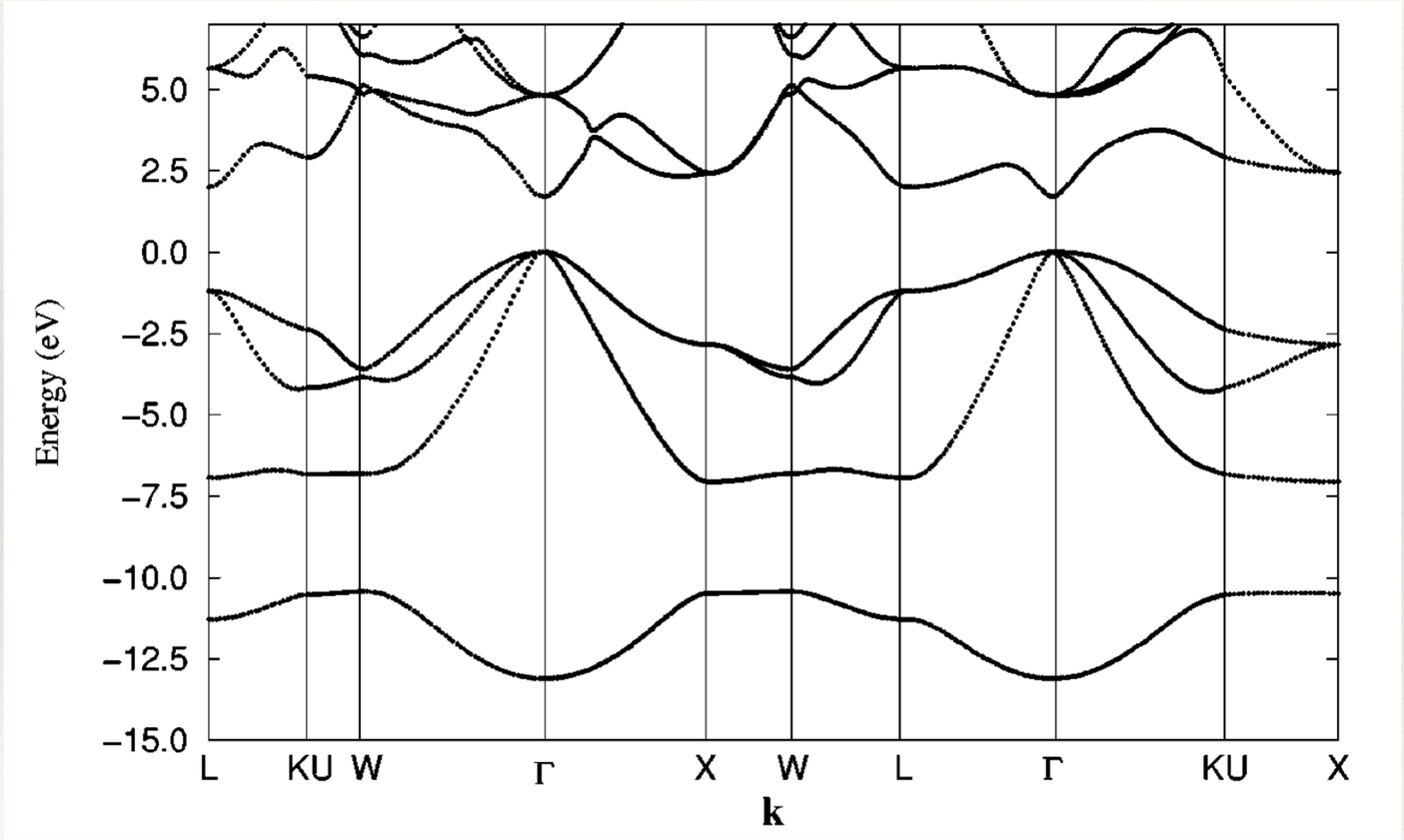


Band-gap ~ 5 eV
Insulator

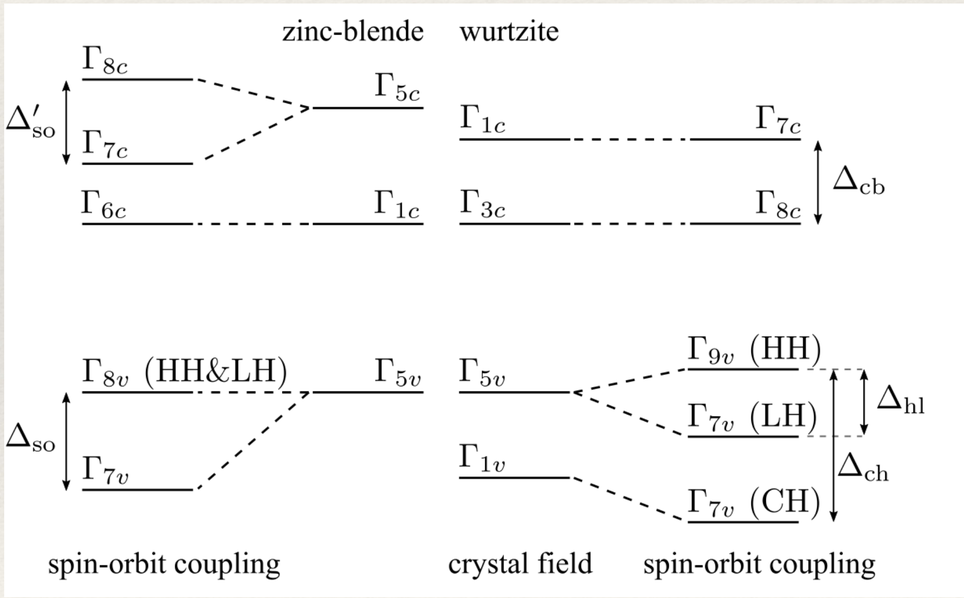
Source: PRB **59**, 5536 (1999)

Typical band structures

GaAs (Zn blende)



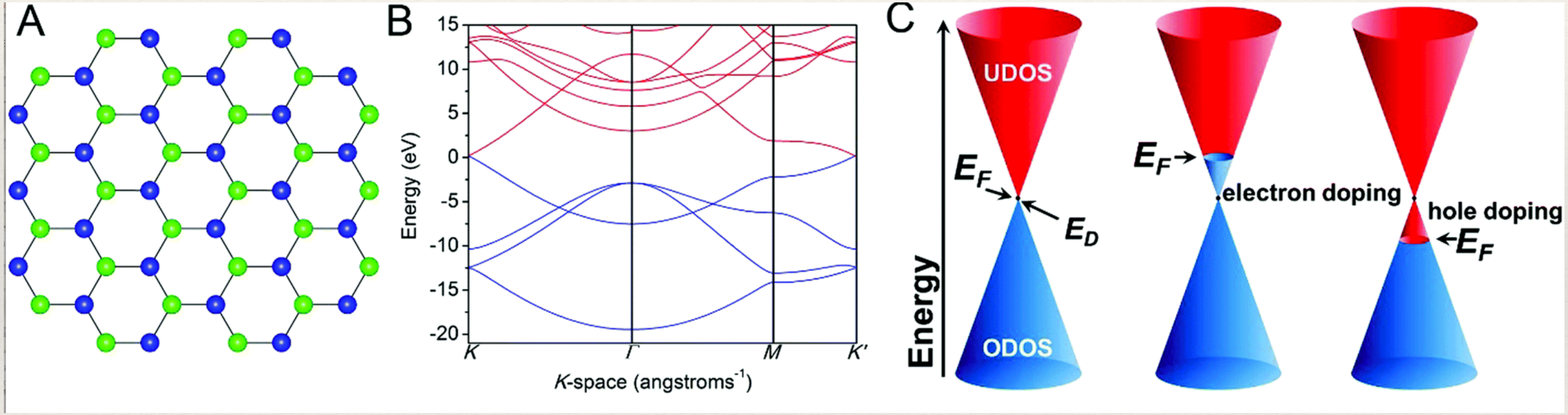
Spin-orbit coupling in valence bands



Source: PRB **59**, 5536 (1999), https://arxiv.org/pdf/1606.00588.pdf

Typical band structures

C (Graphene)



Linear dispersion at K point related some very interesting properties

Source: PRB **59**, 5536 (1999), https://arxiv.org/pdf/1606.00588.pdf