MSE 423 Fall 2024 – Week 9

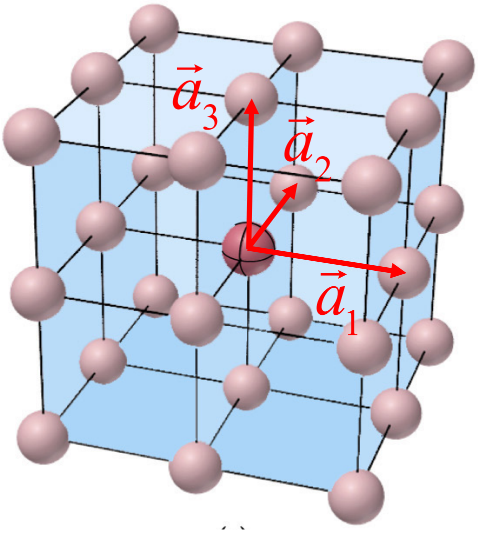
Bloch by Bloch

Last week

- Homonuclear diatomic levels
- Empirical tight binding/Hückel model
- Energy levels and molecular orbitals of benzene
- Symmetry to classify solutions (e.g. in benzene)
- Solutions and spectra in rings
- Symmetry operations, group theory
- Translational symmetry, Bravais lattices
- A crystal as a Bravais lattice + basis
- Primitive, conventional, Wigner-Seitz unit cell

Reciprocal lattice (I)

- Let's start with a Bravais lattice, defined in terms of its primitive lattice vectors…



$$\vec{R} = l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3$$

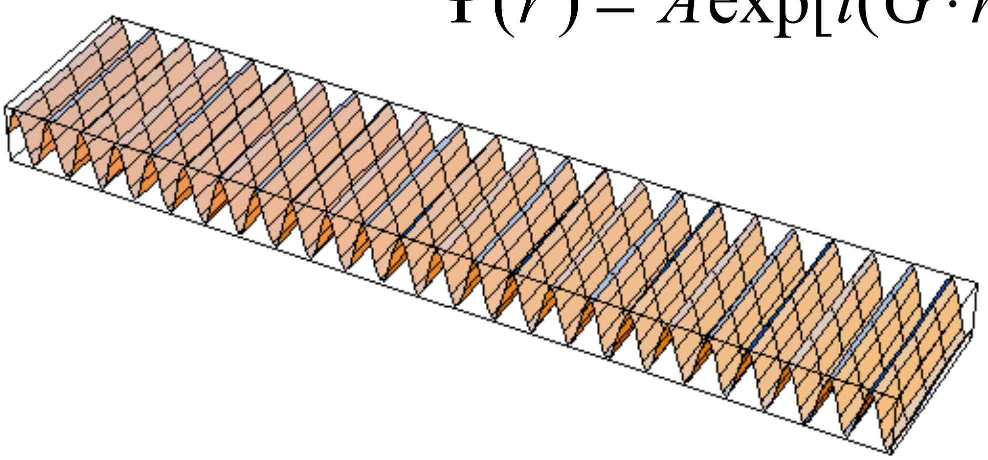
l, m, n integer numbers

$$\vec{R} = (l, m, n)$$

Reciprocal lattice (II)

- …and then let's take a plane wave

$$\Psi(\vec{r}) = A\exp[i(\vec{G}\cdot\vec{r})]$$



Reciprocal lattice (III)

- What are the wavevectors for which our plane wave has the same amplitude at all lattice points ?

$$\exp[i(\vec{G}\cdot\vec{r})] = \exp[i(\vec{G}\cdot(\vec{r}+\vec{R}))]$$
$$\exp[i(\vec{G}\cdot\vec{R})] = 1$$
$$\exp[i(\vec{G}\cdot(l\vec{a}_1 + m\vec{a}_2 + n\vec{a}_3))] = 1$$

$\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ define the primitive unit cell

Reciprocal lattice (IV)

$\vec{G}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$ n integer is satisfied by

$\vec{G} = h\vec{b}_1 + i\vec{b}_2 + j\vec{b}_3$ with h, i, j integers,

provided $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$ $\vec{b}_2 = 2\pi \dfrac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$ $\vec{b}_3 = 2\pi \dfrac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$

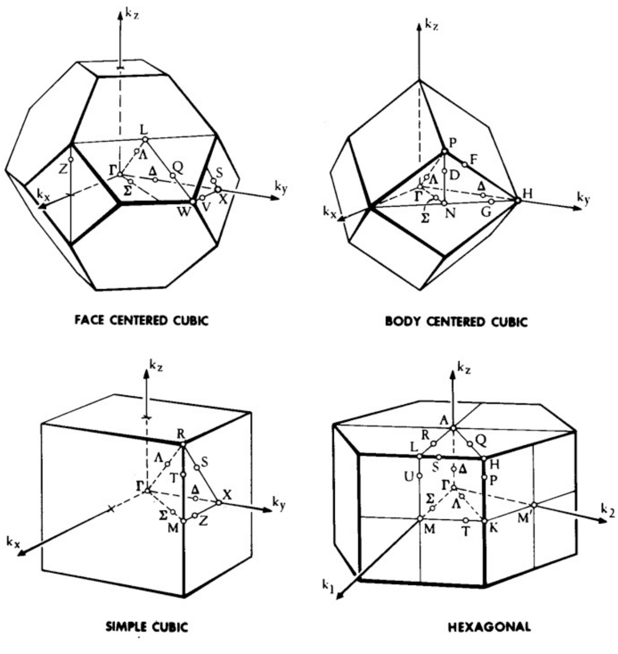
$\vec{G} = (h, i, j)$ are the reciprocal-lattice vectors

Examples of reciprocal lattices

Direct lattice	Reciprocal lattice
Simple cubic	Simple cubic
FCC	BCC
BCC	FCC
Orthorhombic	Orthorhombic

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

Brillouin zones



Brillouin zones are the Wigner-Seitz unit cells of the reciprocal lattice

https://www.materialscloud.org/work/tools/seekpath

Hamiltonian in a periodic potential

Periodic potential

Bloch Theorem

The one-particle effective Hamiltonian $\hat{H}$ in a periodic lattice commutes with the lattice-translation operator $\hat{T}_{\mathrm{R}}$, allowing us to choose the common eigenstates according to the prescriptions of Bloch theorem:

$$[\hat{H}, \hat{T}_{\mathrm{R}}] = 0 \quad \Rightarrow \quad \Psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}}$$

- n, k are the quantum numbers (band index and crystal momentum), u is periodic
- From two requirements: a translation can't change the charge density, and two translations must be equivalent to one that is the sum of the two

Bloch Theorem

Bloch Theorem

Bloch Theorem

Bloch Theorem (in two equiv forms)

$$\Psi_{\vec{k}}\left(\vec{r}+\vec{R}\right)=\exp\left(i\vec{k}\cdot\vec{R}\right)\Psi_{\vec{k}}\left(\vec{r}\right)$$

Bloch Theorem (in two equiv forms)

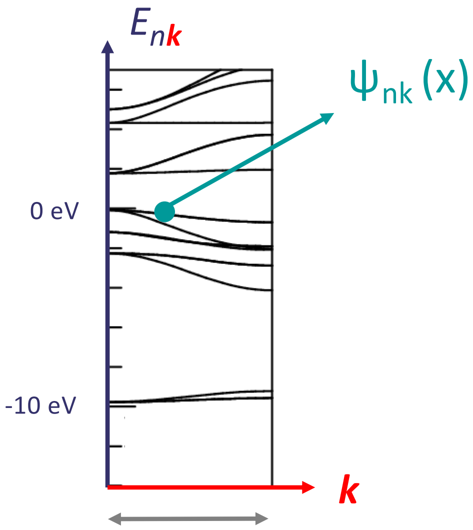
$$\Psi_{\vec{k}}\left(\vec{r}+\vec{R}\right)=\exp\left(i\vec{k}\cdot\vec{R}\right)\Psi_{\vec{k}}\left(\vec{r}\right)$$

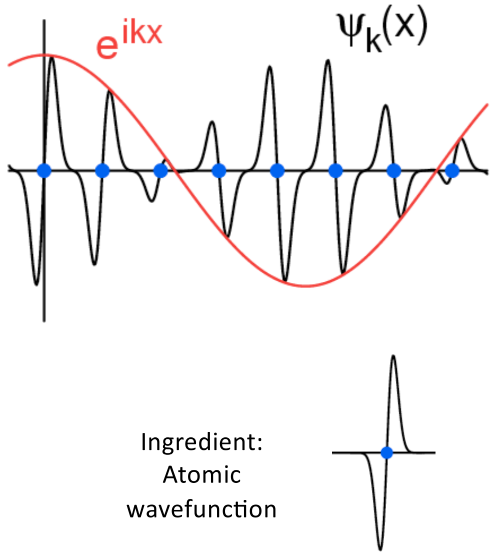
$$\Psi_{\vec{k}}\left(\vec{r}\right)=\exp\left(i\vec{k}\cdot\vec{r}\right)u_{\vec{k}}\left(\vec{r}\right)$$

MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2024)

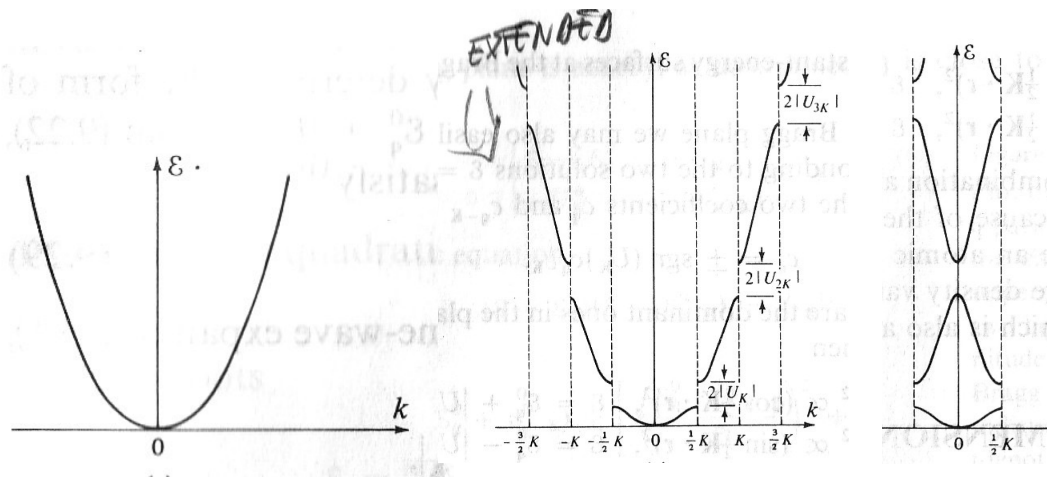
Bloch Theorem

Bloch wavefunction

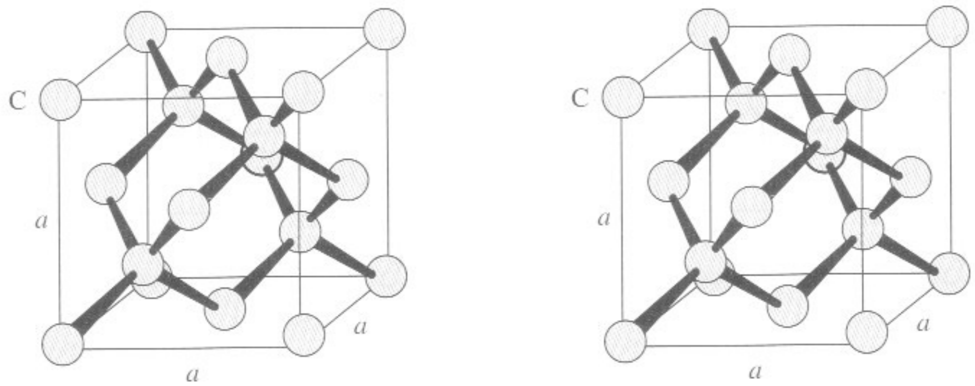




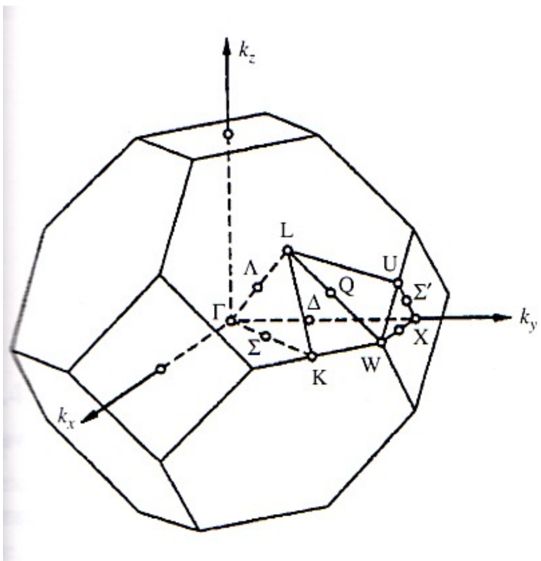
From extended to primitive



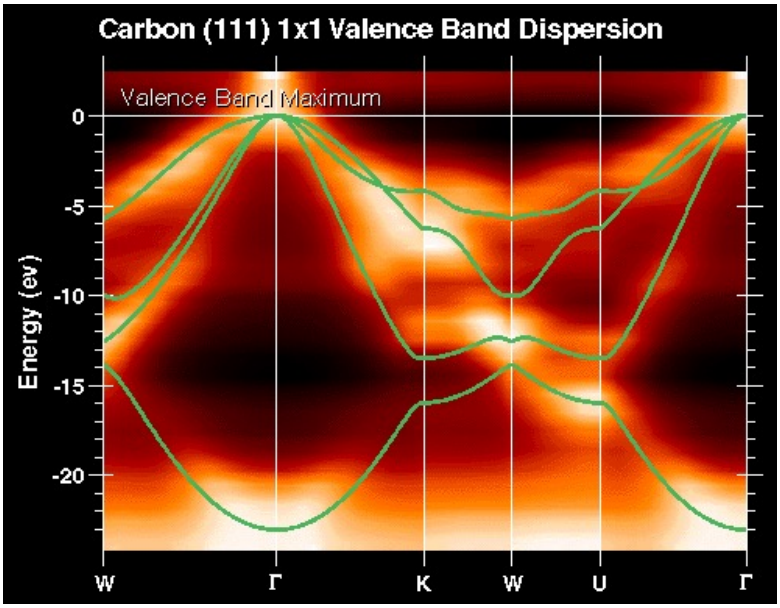
Diamond and Zincblend



Brillouin Zone (fcc)

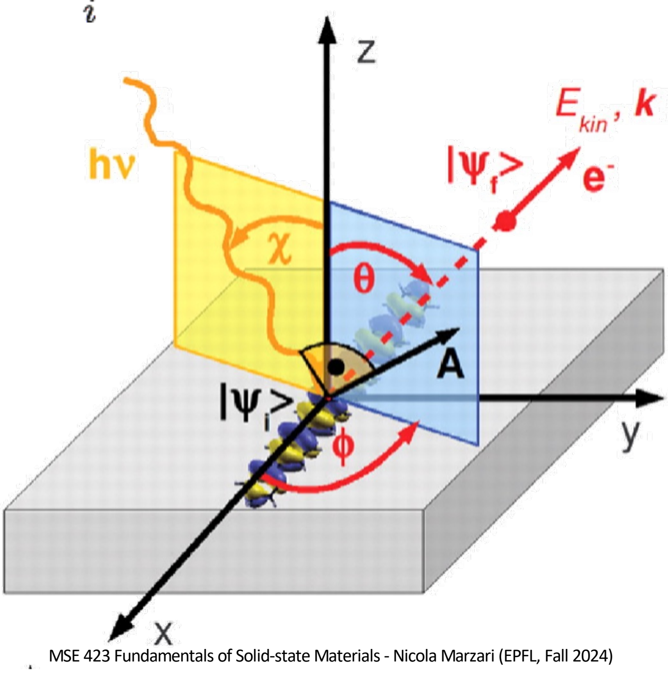


Band Structure of Diamond

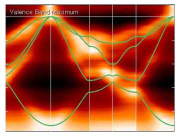


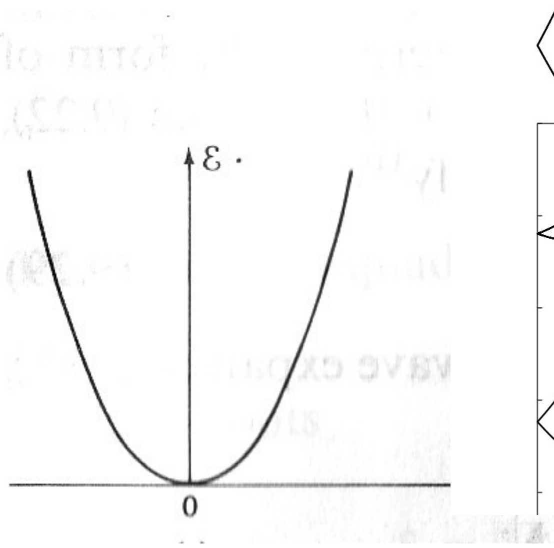
ARPES: Angle resolved photoemission spectroscopy

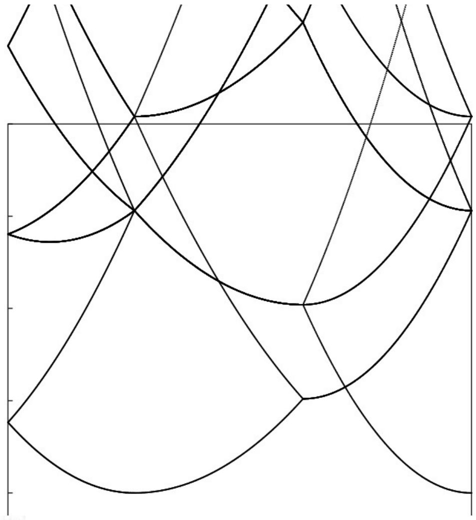
$$I(\omega) = \sum_i |\langle \varphi_f | \hat{H}_{\text{int}} | \varphi_i \rangle|^2 \delta(\epsilon_f - \epsilon_i - \hbar\omega)$$



Why does it look like this?







Band Structures: Free Electron Gas, Silicon