Introduction to Wannierization
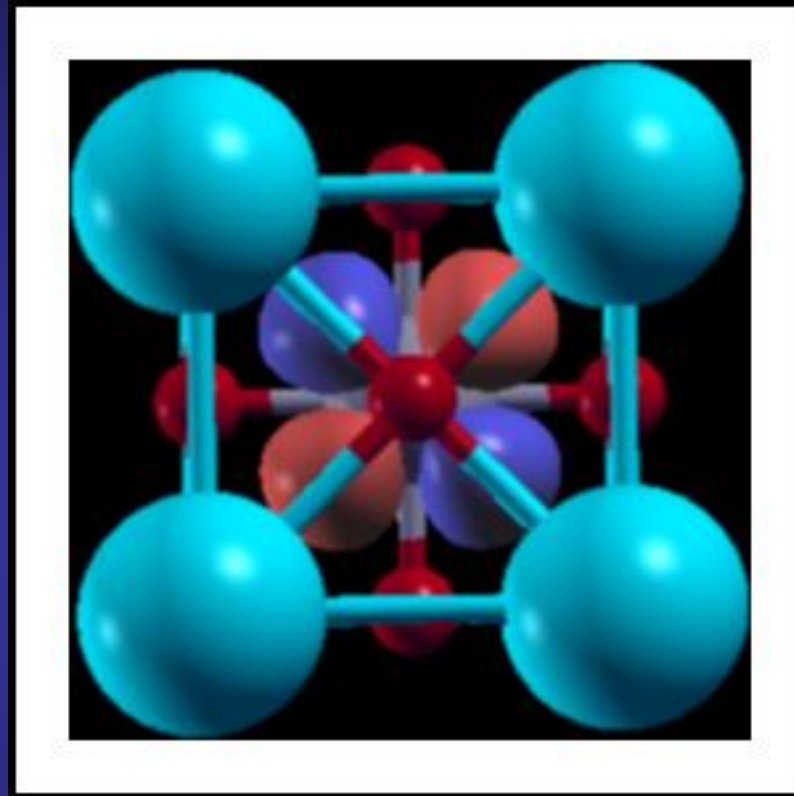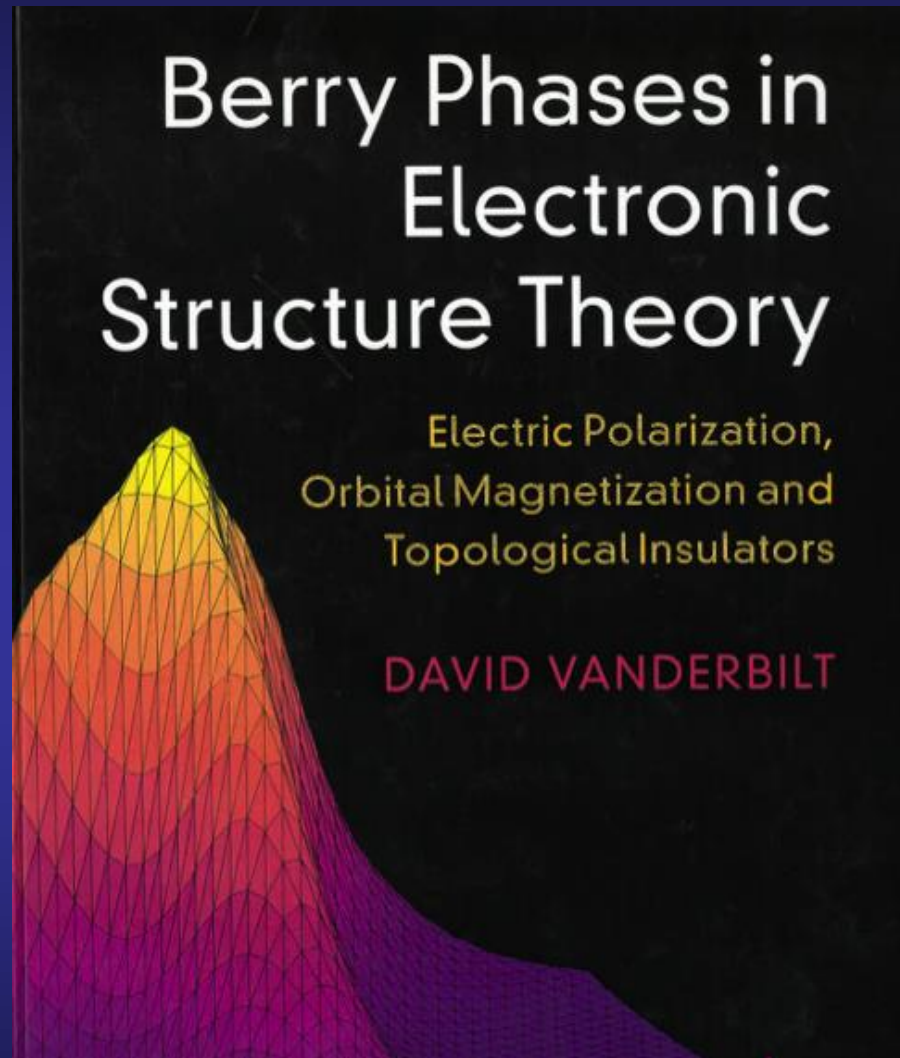

Javier Junquera

Most important references followed in this lecture

Important bibliography:

For a review on Maximally Localized Wannier functions:

Maximally localized Wannier functions: Theory and applications

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Outline

Definition

Basic properties

Potential uses

Maximally Localized Wannier Functions

Wannierization in SIESTA

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Definition

Basic properties
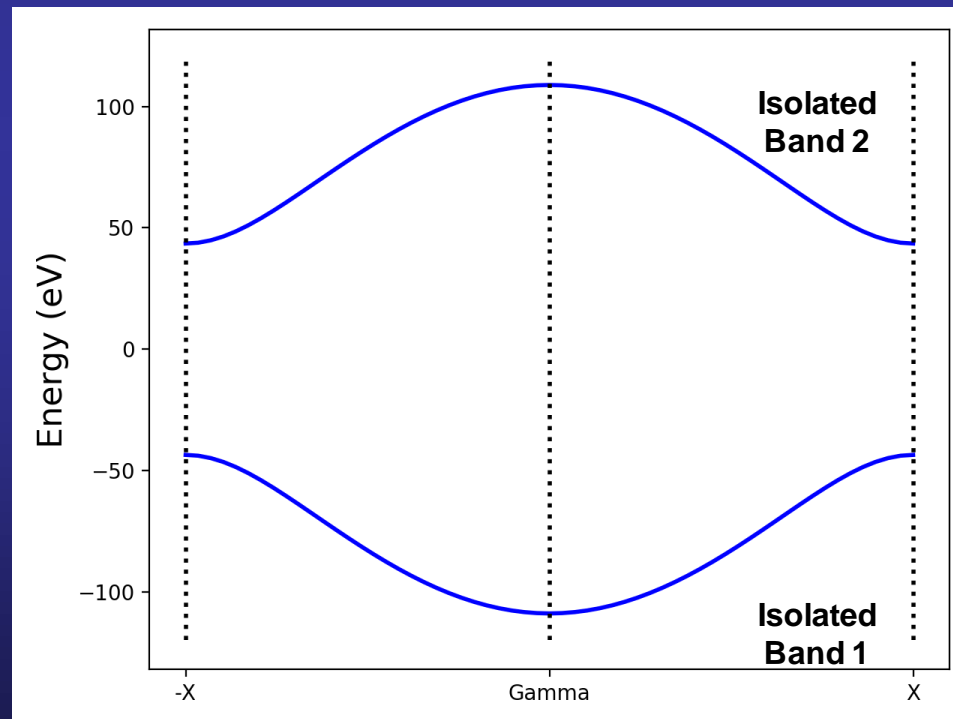
Potential uses

Maximally Localized Wannier Functions

Wannierization in SIESTA

Wannier functions in isolated bands

Let us assume that we have isolated bands $E_n(\vec{k})$ meaning that they never touch the bands below or above them

We can assume that $E_n(\vec{k})$ are smooth, continuous and periodic functions in $\vec{k}$ in the 3D reciprocal space

Wannier functions in isolated bands

Let us assume that we have isolated bands $E_n(\vec{k})$ meaning that they never touch the bands below or above them

We can assume that $E_n(\vec{k})$ are smooth, continuous and periodic functions in $\vec{k}$ in the 3D reciprocal space

Then, it is natural to consider its Fourier transform in real space

$$E_{n\vec{R}} = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}} E_{n\vec{k}} \; d^3k \iff E_{n\vec{k}} = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} E_{n\vec{R}}$$

FFT

If $E_n(\vec{k})$ is smooth in $\vec{k}$ space, we can expect to be large only for a few lattice vectors $\vec{R}$ near the origin, and decay rapidly with increasing $|\vec{R}|$
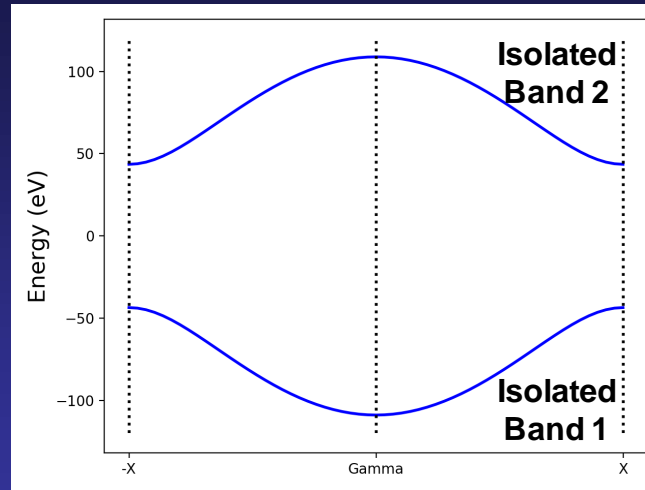
Wannier functions in isolated bands
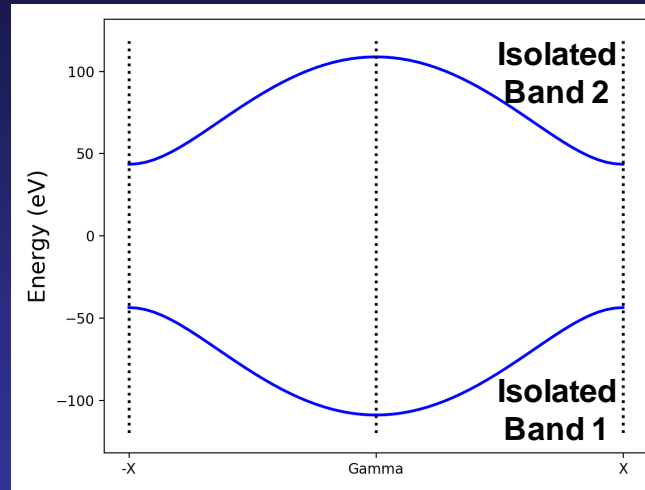
We can **choose** a smooth and periodic gauge for the Bloch functions $|\psi_{n\vec{k}}\rangle$ associated with each band

The Fourier-transform partners of the Bloch functions are known as Wannier functions associated with band n

$$|w_{n\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}} |\psi_{n\vec{k}}\rangle d^3k \quad \underset{\text{FFT}}{\Longleftrightarrow} \quad |\psi_{n\vec{k}}\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} |w_{n\vec{R}}\rangle$$

As long as $\psi_{n\vec{k}}(\vec{r})$ is a **smooth function of** $\vec{k}$, then $w_{n\vec{R}}(\vec{r})$ decays rapidly with $|\vec{R}|$ for a given $\vec{r}$.

Wannier functions in isolated bands

We can **choose** a smooth and periodic gauge for the Bloch functions $|\psi_{n\vec{k}}\rangle$ associated with each band

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$$|w_{n\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}}|\psi_{n\vec{k}}\rangle d^3k \iff_{\textbf{FFT}} |\psi_{n\vec{k}}\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}|w_{n\vec{R}}\rangle$$

This is an special case of an **unitary transformation**

We can view the Bloch and Wannier functions as providing two different basis sets describing the same manifold of states associated with the electron band in question

Wannier functions in isolated bands

The Fourier-transform partners of the Bloch functions are known as Wannier functions
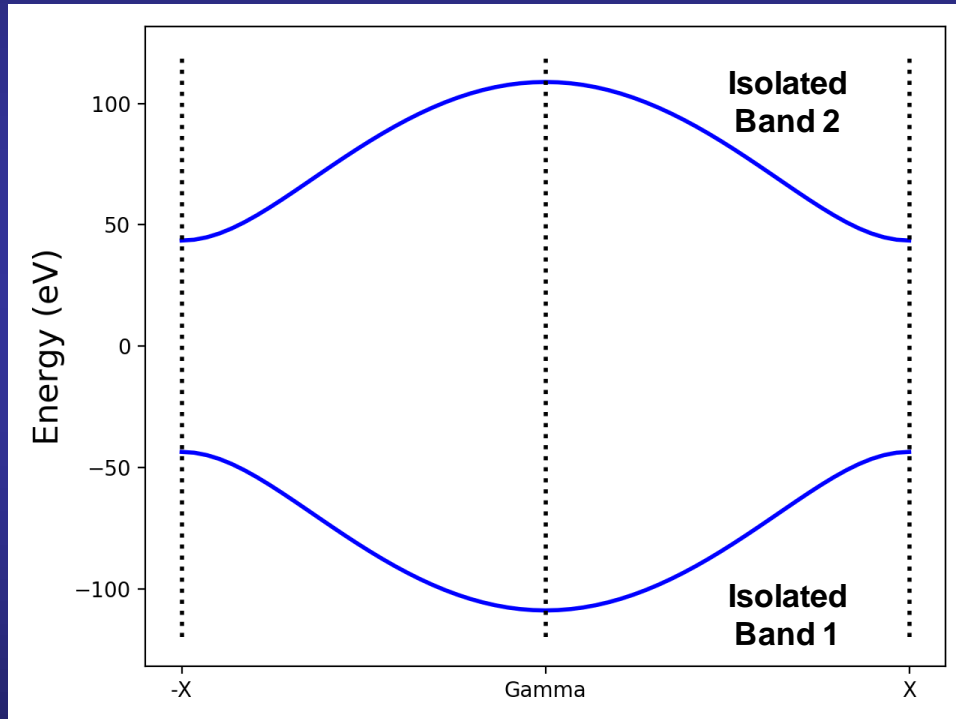
$$|w_{2\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}}|\psi_{2\vec{k}}\rangle d^3k$$

$$|w_{1\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}}|\psi_{1\vec{k}}\rangle d^3k$$

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Properties of the Wannier functions in the single band case

1. They are localized functions in real space

$$\left| w_{n\vec{R}}(\vec{r}) \right| \longrightarrow 0 \text{ as } \left| \vec{r} - \vec{R} \right| \text{ gets large}$$

Each Wannier function $w_{n\vec{R}}(\vec{r})$ is a localized function centered near $\vec{R}$, so it is more natural to describe the situaton by saying that $w_{n\vec{R}}(\vec{r})$ decays rapidly with $\left| \vec{r} - \vec{R} \right|$

Properties of the Wannier functions in the single band case

2. The Wannier functions are translational images of one another

$$w_{n\vec{R}}(\vec{r}) = w_{n\vec{0}}(\vec{r} - \vec{R})$$

Or more formally

$$|n\vec{R}\rangle = T_{\vec{R}}|n\vec{0}\rangle$$

$T_{\vec{R}}$ **is the operator that translates the system by a lattice vector** $\vec{R}$

Properties of the Wannier functions
in the single band case

3. The Wannier functions form an orthonormal set

Single band case

$$\langle w_{n\vec{R}} | w_{n\vec{R'}} \rangle = \delta_{\vec{R}\vec{R'}}$$

Properties of the Wannier functions in the single band case

4. The Wannier functions span the same subspace of the Hilbert space as is spanned by the Bloch functions from which they are constructed
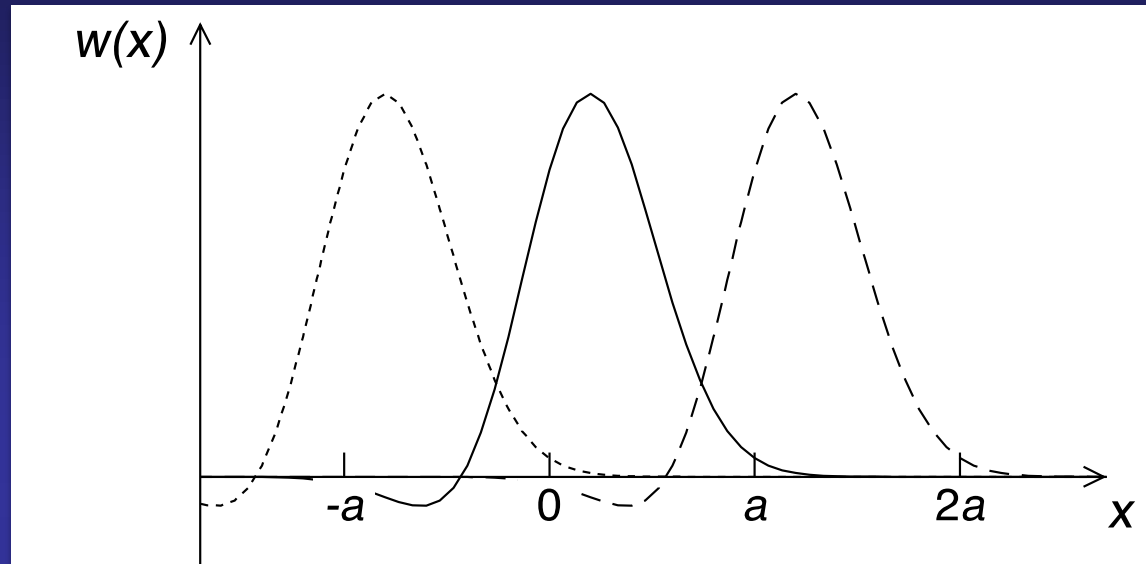
Single band case

Let $\mathcal{P}_n$ be the projector operator on band n then this can be expressed as

$$\mathcal{P}_n = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} |\psi_{n\vec{k}}\rangle\langle\psi_{n\vec{k}}| d^3k = \sum_{\vec{R}} |w_{n\vec{R}}\rangle\langle w_{n\vec{R}}|$$

From this it follows that the total charge density $\rho_n(\vec{r})$ in band n is the same when computed in every representation

$$\rho_n(\vec{r}) = -e\langle\vec{r}|\mathcal{P}_n|\vec{r}\rangle = -e\frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} |\psi_{n\vec{k}}(\vec{r})|^2 d^3k = -e\sum_{\vec{R}} |w_{n\vec{R}}(\vec{r})|^2$$

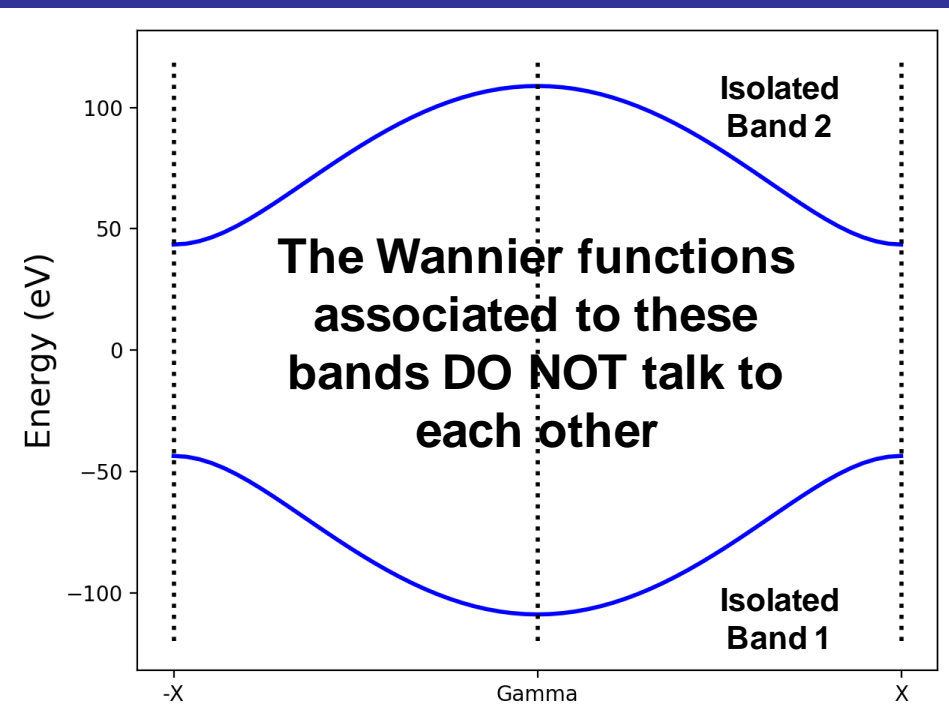# Properties of the Wannier functions in the single band case

Example in 1D

- **Exponentially localized**
- **Normalized**
- **Neighboring Wannier functions are periodic images of one another**
- **They are shown as having a negative lobe so that $\langle w_{n0} | w_{na} \rangle$ vanish as a result of the cancellation between contributions of opposite sign in the integral over x**

The Hamiltonian matrix elements between Wannier functions are band-diagonal

$$\langle w_{m\vec{R}}|H|w_{n\vec{R'}}\rangle = 0 \qquad \text{if} \qquad n \neq m$$

In the previous example

$$\langle w_{1\vec{R}}|H|w_{2\vec{R'}}\rangle = 0$$

The Wannier functions associated to these bands DO NOT talk to each other

$$|w_{2\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3}\int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}}|\psi_{2\vec{k}}\rangle d^3k$$

$$|w_{1\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3}\int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}}|\psi_{1\vec{k}}\rangle d^3k$$

The diagonal elements of the Hamiltonian matrix elements between Wannier functions are the coefficients in the Fourier expansion of the band energy

$$\langle w_{n\vec{0}}|H|w_{n\vec{R}}\rangle = E_{n\vec{R}}$$

where

$$E_{n\vec{R}} = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}} E_{n\vec{k}} \; d^3k$$

From the knowledge of:
- **the band structure**
- **The k-point mesh**
- **The unit cell volumen**

We get the values of the Hamiltonian matrix written in a basis of Wannier functions

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The Wannier functions provide an exact tight-binding representation of the dispersion $E_{n\vec{k}}$ of band n

The Fourier components of the energy can be considered as the on-site and hopping elements of a tight-binding Hamiltonian

Here we show three periodic replicas and their corresponding Wannier centers
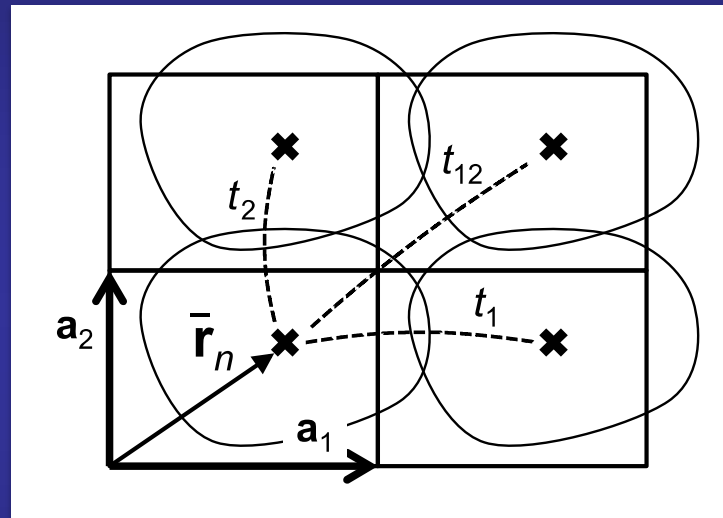
The hoppings correspond to

$$t_1 \rightarrow E_{n,\vec{a}_1}$$

$$t_2 \rightarrow E_{n,\vec{a}_2}$$

$$t_{12} \rightarrow E_{n,\vec{a}_1+\vec{a}_2}$$

$E_{n\vec{0}}$ **is the on-site energy**

The tight-binding equations are nothing else that the expression of the inverse Fourier transform for the energy terms

$$\tilde{H}_{ij}(\vec{k}) = \langle \tilde{\chi}_i(\vec{k})|H|\tilde{\chi}_j(\vec{k})\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} H_{ij}(\vec{R}) \qquad \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} E_{n\vec{R}} = E_{n\vec{k}}$$

And, by construction, it reproduces exactly the band dispersion

Wannier interpolation: approach of keeping only a few hoppings

Since the Wannier functions are localized,
the hopping matrix elements decay rapidly with distances,
so that a few hoppings are tipically retained

$$E_{n\vec{k}} \approx \sum_{\substack{\vec{R} \\ |\vec{R}| < R_c}} e^{i\vec{k}\cdot\vec{R}} E_{n\vec{R}}$$

If these are the dominant hoppings, this simple model may be expected to provide a good approximation to the full band structure.
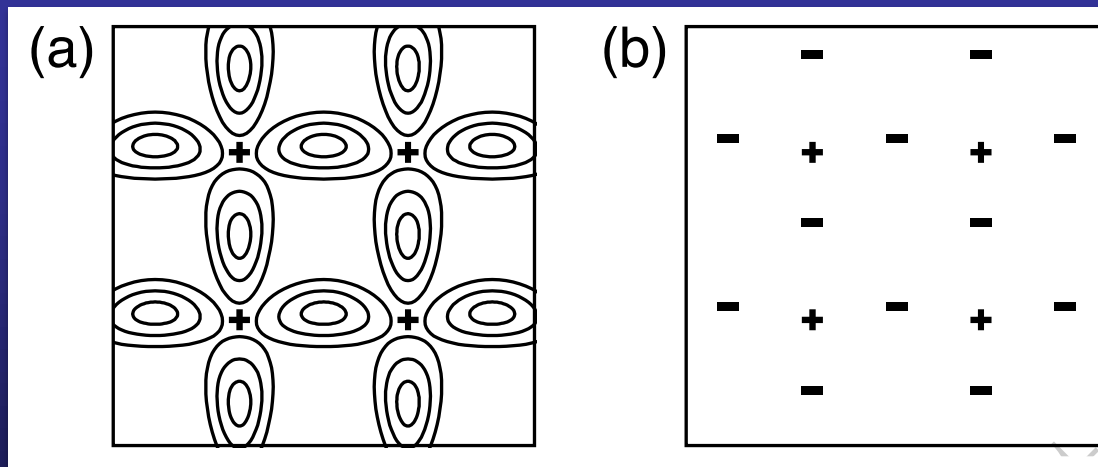
But the model is guaranteed to become more and more accurate as farther–neighbor hoppings are added

Relationship between Wannier centers and Berry phase polarization (isolated bands)

The electronic contribution to the polarization is determined entirely by the Wannier centers of the occupied bands

$$\vec{P} = \frac{-e}{V_{\text{cell}}} \sum_{n}^{\text{occ}} \bar{\vec{r}}_n$$

$$\bar{\vec{r}}_n = \langle w_{n\vec{0}} | \vec{r} | w_{n\vec{0}} \rangle$$

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Wannier functions are not unique

$$|w_{n\vec{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\vec{k}\cdot\vec{R}} |\psi_{n\vec{k}}\rangle d^3k \iff |\psi_{n\vec{k}}\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} |w_{n\vec{R}}\rangle$$

FFT

- **Many different gauge transformations to chose the phases of the Bloch functions are possible**

As a result, the Wannier functions may change shape, becoming somewhat more or less localized

Maximally localized Wannier function

How to chose a sensible gauge for the computation of the Wannier functions

Criterion of maximal localization:
minimize the sum of spreads of the Wannier functions in one unit cell

$$\Omega_{\text{spread}} = \sum_{n=1}^{J} \left[\langle w_{n\vec{0}} | r^2 | w_{n\vec{0}} \rangle - |\vec{\bar{r}}_n|^2 \right]$$

↑

**Mean square variation of the Wannier
electron density away from its mean position**

N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)

This is the criterion followed in WANNIER90

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Interface between SIESTA and WANNIER90

http://www.wannier.org

Wannier90 as a community code: new features and applications

Giovanni Pizzi[1,29,30], Valerio Vitale[2,3,29], Ryotaro Arita[4,5],
Stefan Blügel[6], Frank Freimuth[6], Guillaume Géranton[6],
Marco Gibertini[1,7], Dominik Gresch[8], Charles Johnson[9],
Takashi Koretsune[10,11], Julen Ibañez-Azpiroz[12], Hyungjun Lee[13,14],
Jae-Mo Lihm[15], Daniel Marchand[16], Antimo Marrazzo[1],
Yuriy Mokrousov[6,17], Jamal I Mustafa[18], Yoshiro Nohara[19],
Yusuke Nomura[4], Lorenzo Paulatto[20], Samuel Poncé[21],
Thomas Ponweiser[22], Junfeng Qiao[23], Florian Thöle[24],
Stepan S Tsirkin[12,25], Małgorzata Wierzbowska[26], Nicola Marzari[1,29],
David Vanderbilt[27,29], Ivo Souza[12,28,29], Arash A Mostofi[3,29]
and Jonathan R Yates[21,29]

Can be run as:
- **Postprocessing tool**
- **As a library within SIESTA (coming son).**

Requirements to feed WANNIER90 from SIESTA

SIESTA **must compute:**

The overlap of the periodic part of the wave functions at neighbour k-points

$$M_{mn}^{(\vec{k},\vec{b})} = \langle u_{m\vec{k}} | u_{n\vec{k}+\vec{b}} \rangle$$

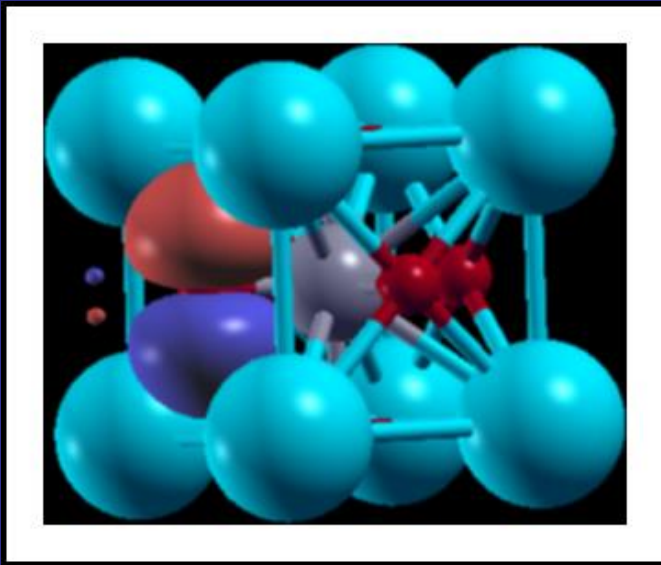$\vec{b}$ **is the vector which connect a given** $\vec{k}$ **with its neighbours**

The overlap of the Bloch states $|\psi_{m\vec{k}}\rangle$ **onto trial localised orbitals** $|g_n\rangle$

$$A_{mn}^{(\vec{k})} = \langle \psi_{m\vec{k}} | g_n \rangle$$

The eigenvalues of the Hamiltonian in grid of k-points

Exercise 1: Wannierize the top of the valence band and the bottom of the conduction band of $SrTiO_3$
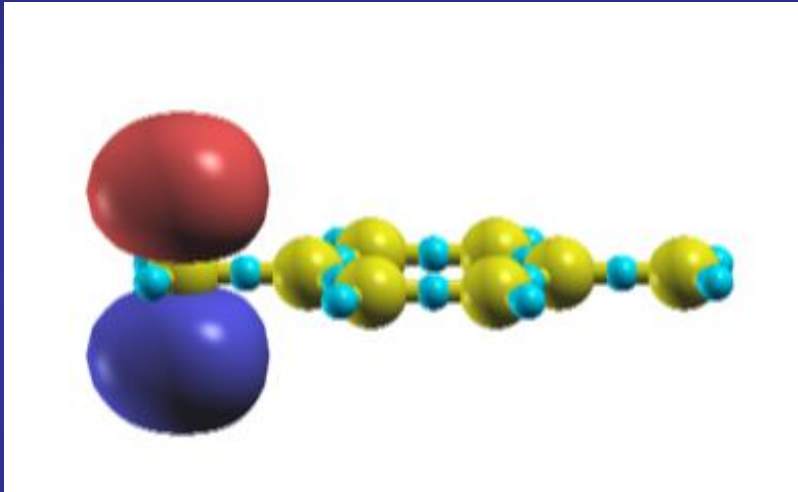
Top of valence band

O 2p in character
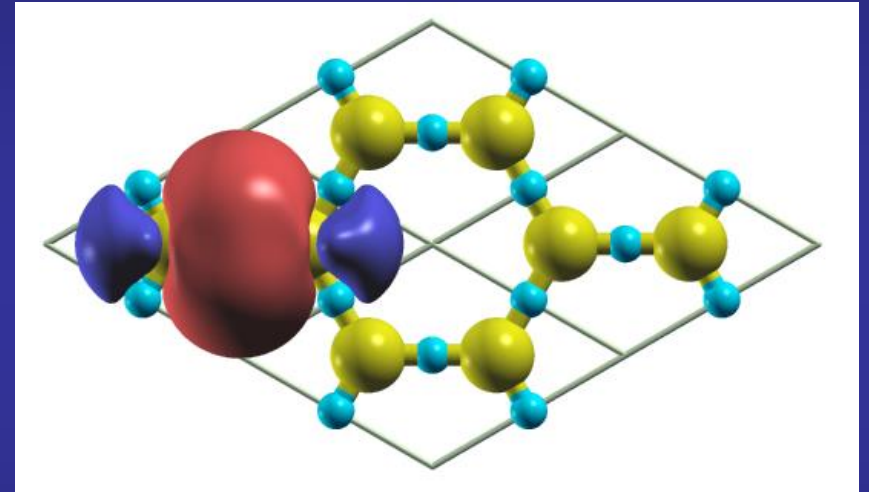
Bottom of conduction band
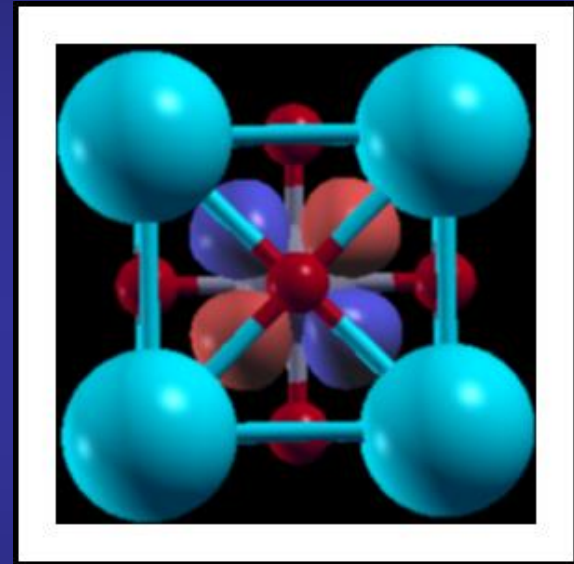
Ti t_{2g} in character

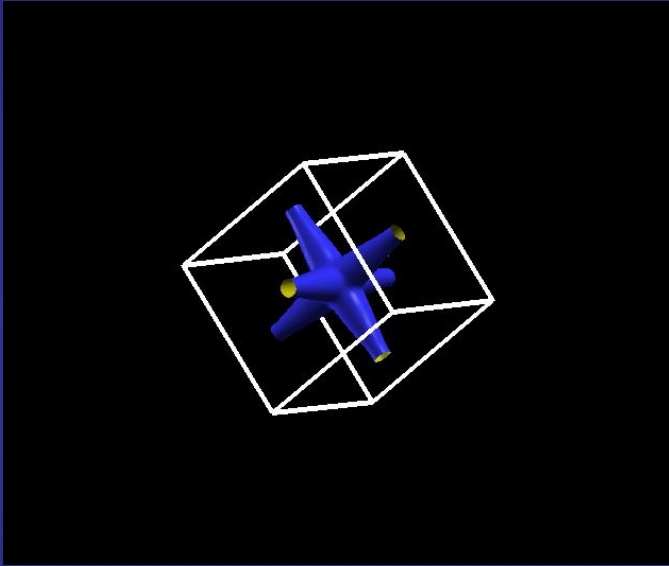# Exercise 2: Wannierize the bands of Graphene (disentanglement)
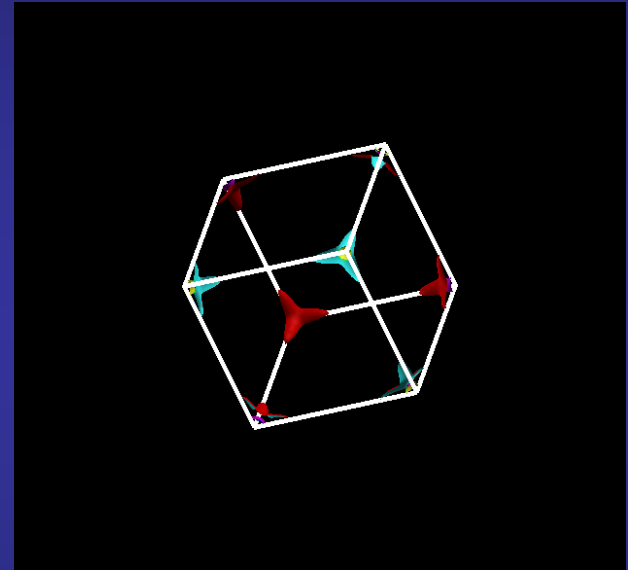

π bonding

σ bonding

Exercise 3: Plotting the Fermi Surface of doped SrTiO$_3$

Doping with electrons

Doping with holes