Practical tight-binding models for Twisted Bilayer Systems. Connection to ab-initio calculations.

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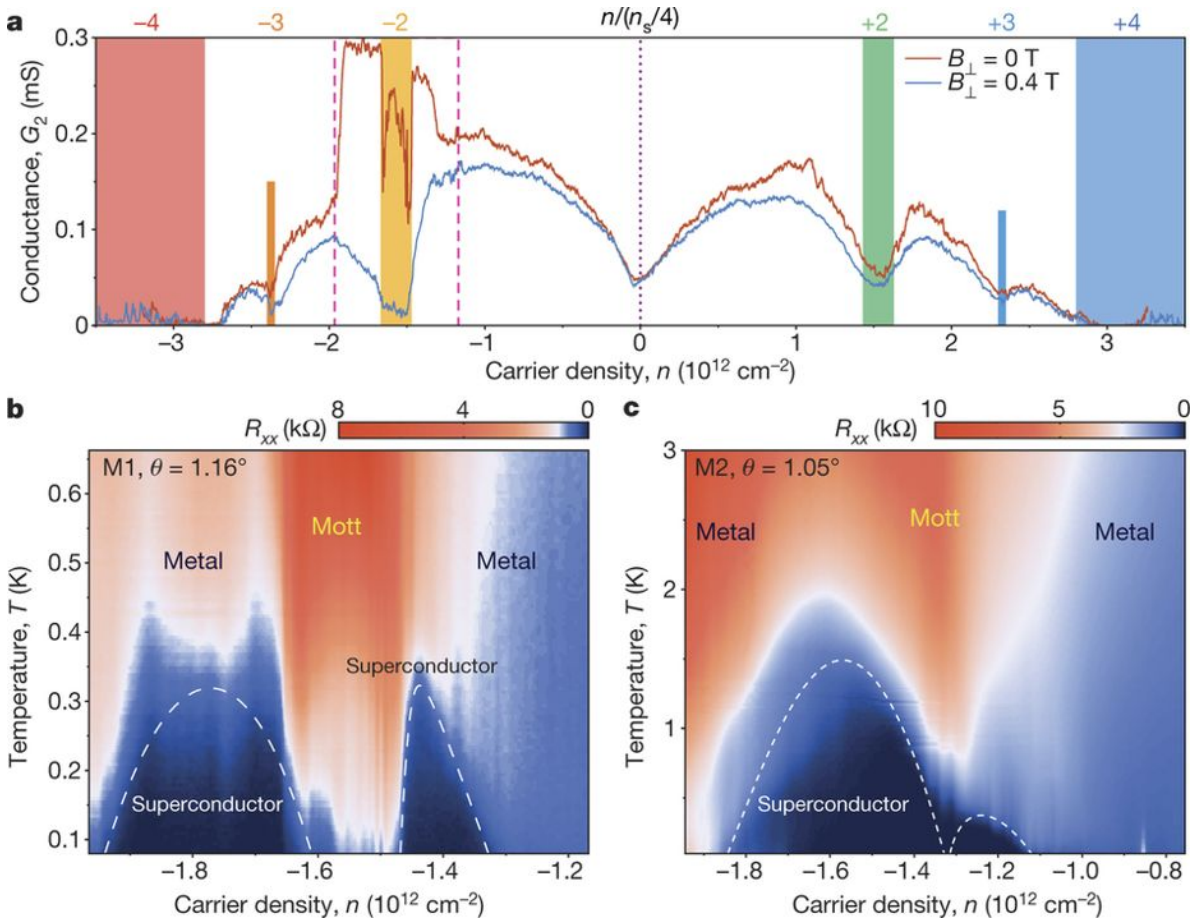
Oct 2019

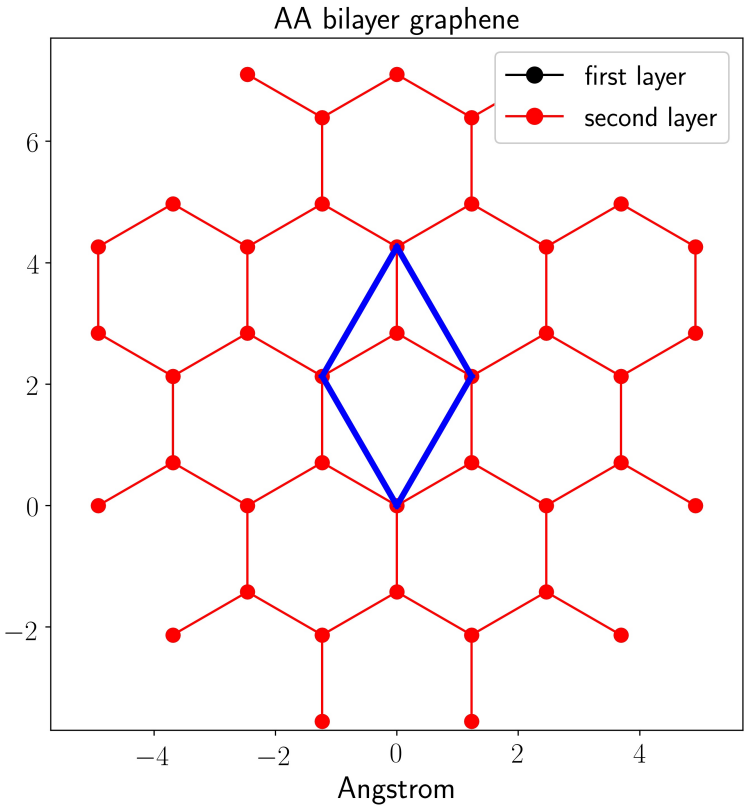
Outline

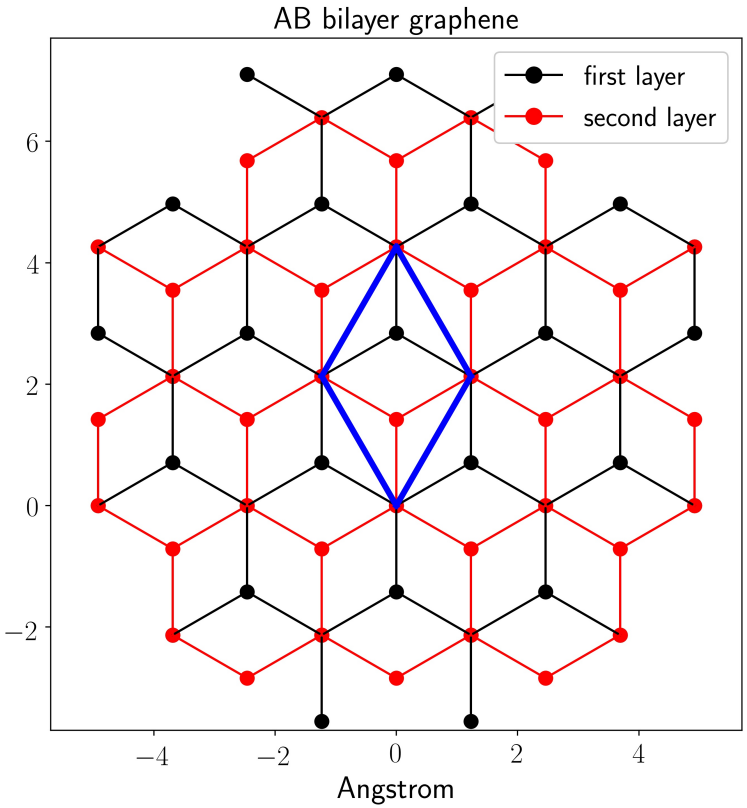
Some physics of TBG



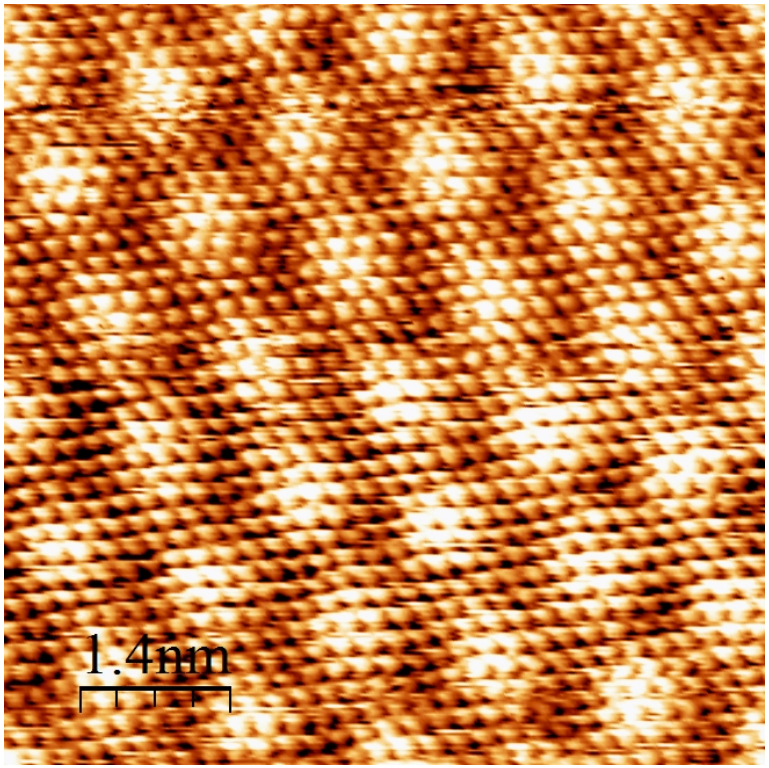
Nature **556**, p. 43–50 (2018)

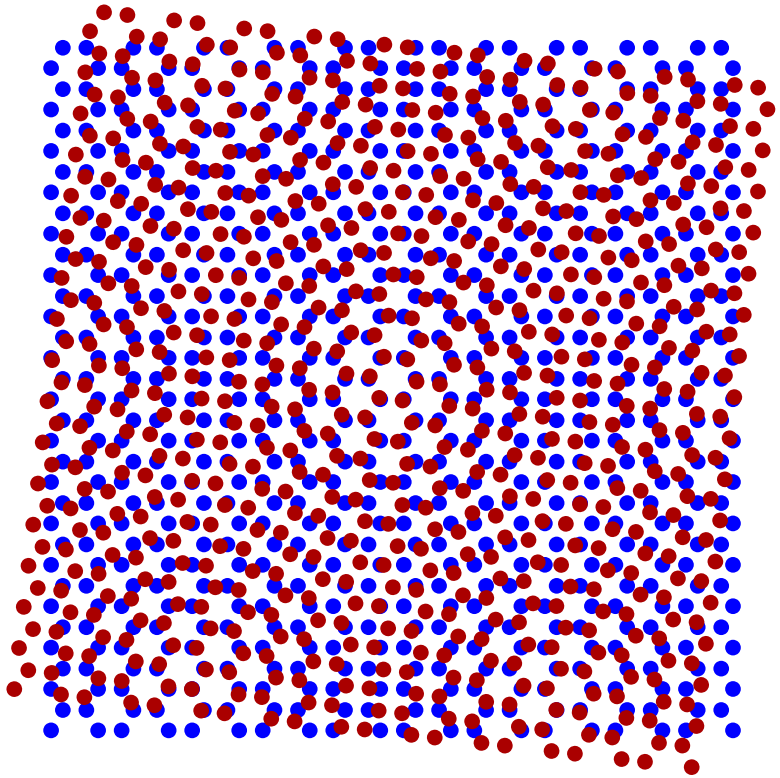
AA and AB double layers of graphene





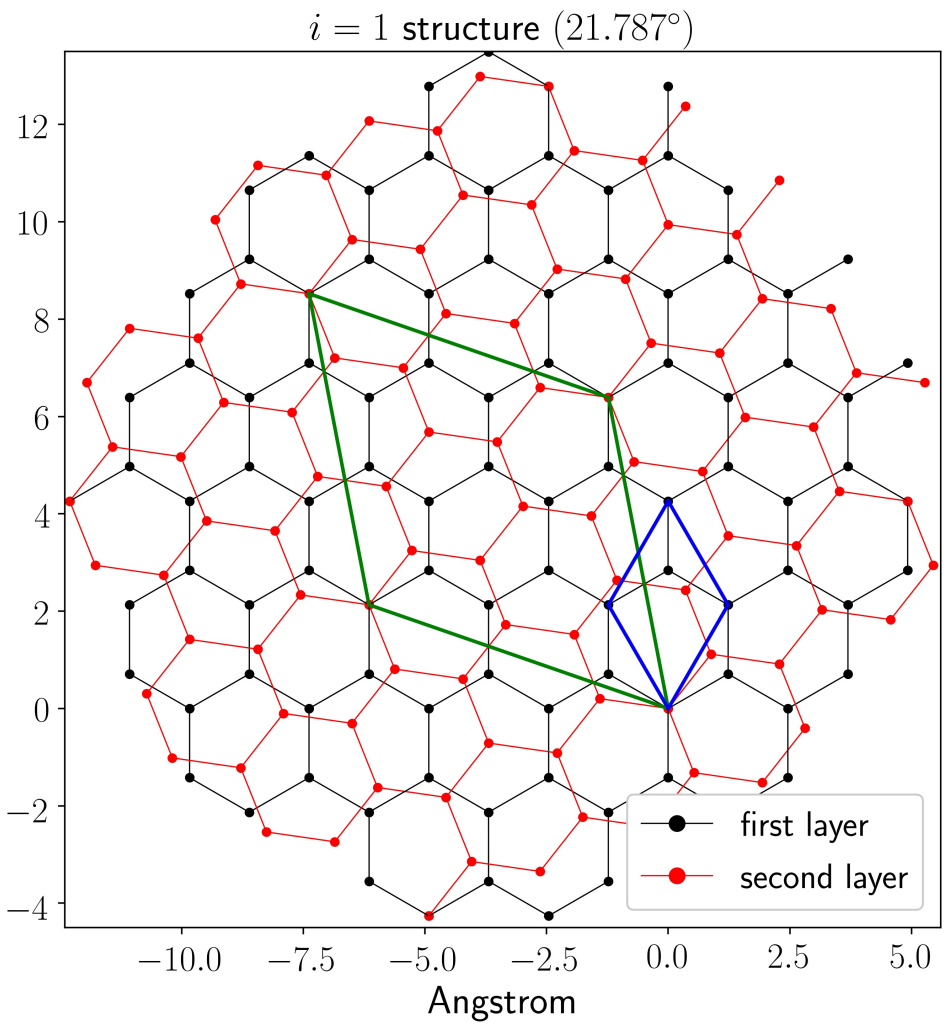
Moiré pattern





STM : Phys. Rev. B 81, 045403

Commensurate : (1)21.79, (2)13.17, . . . , (30)1.08, (31)1.05



Numerical challenge

- Unit cell at magic angle (1.05) contains about 12 thousand atoms
- This results in 2.3×10^9 matrix elements of Hamiltonian on SIESTA's simplest basis, which is around 34 GB per k-point.
- One needs a smaller model/basis set to handle the problem

Tight-binding Hamiltonian

- Single-particle Hamiltonian in localised basis set :

$$H_{nm}(\mathbf{R}) = \langle \varphi_n(\mathbf{r}) | H(\mathbf{r}) | \varphi_m(\mathbf{r} - \mathbf{R}) \rangle$$

  real-space form of Hamiltonian is encoded in a matrix

- At this stage one could get the spectra $\epsilon_{j\mathbf{k}}$:by :

$$(1)\ H_{nm}(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} H_{nm}(\mathbf{R})$$

$$(2)\ \hat{H}_{\mathbf{k}} \vec{C}_{j\mathbf{k}} = \epsilon_{j\mathbf{k}} \vec{C}_{j\mathbf{k}}$$

- Can we substitute $H_{nm}(\mathbf{R})$ with model parameters $t_{nm}(\mathbf{R})$-hopping amplitudes ?

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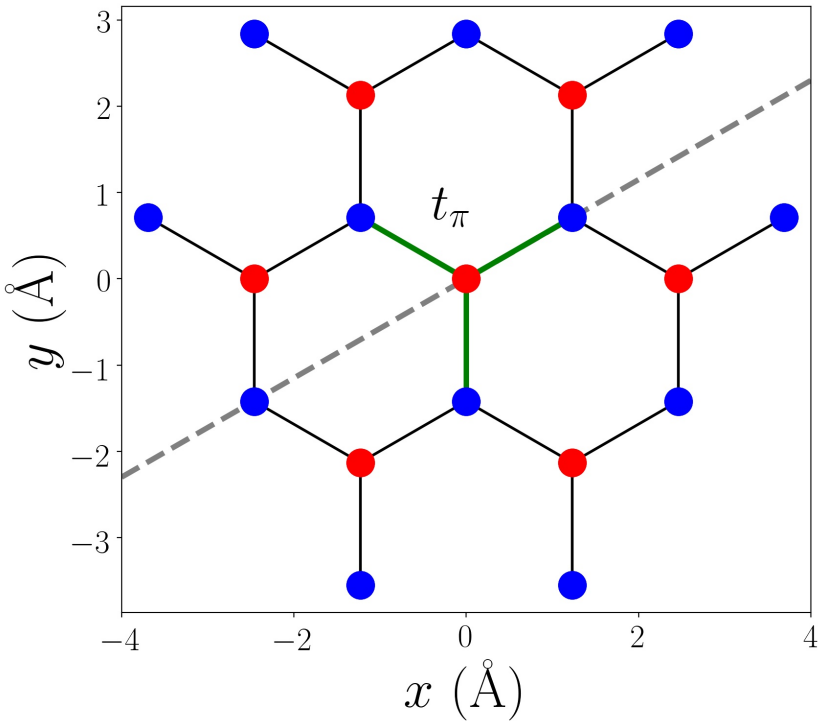
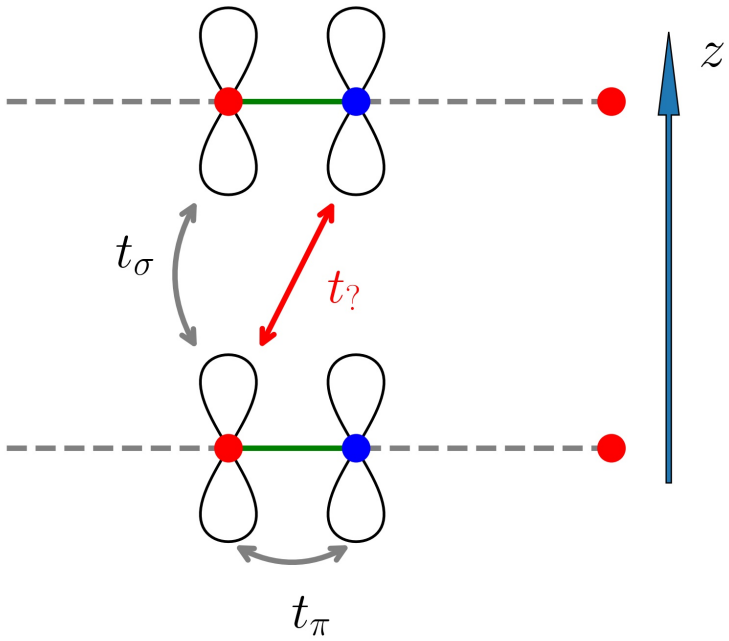
Slater-Koster approach for TBG : one p_z orbital per site





Slater-Koster approach

- Hopping parameters are modulated as a function of vector conecting orbital centers [1] [2] :

$$t_{ij} = t(\mathbf{r}_{ij}) = (1 - n^2)t_\pi(r_{ij}) + n^2 t_\sigma(r_{ij})$$

1. M. Koshino et.al, Phys. Rev. X 8, 031087
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$$\begin{aligned} n &= z_{ij}/r_{ij} \\ t_\pi(r_{ij}) &= t_\pi^0 e^{q_\pi(1-\frac{r_{ij}}{a_\pi})} \\ t_\sigma(r_{ij}) &= t_\sigma^0 e^{q_\sigma(1-\frac{r_{ij}}{a_\sigma})} \end{aligned}$$

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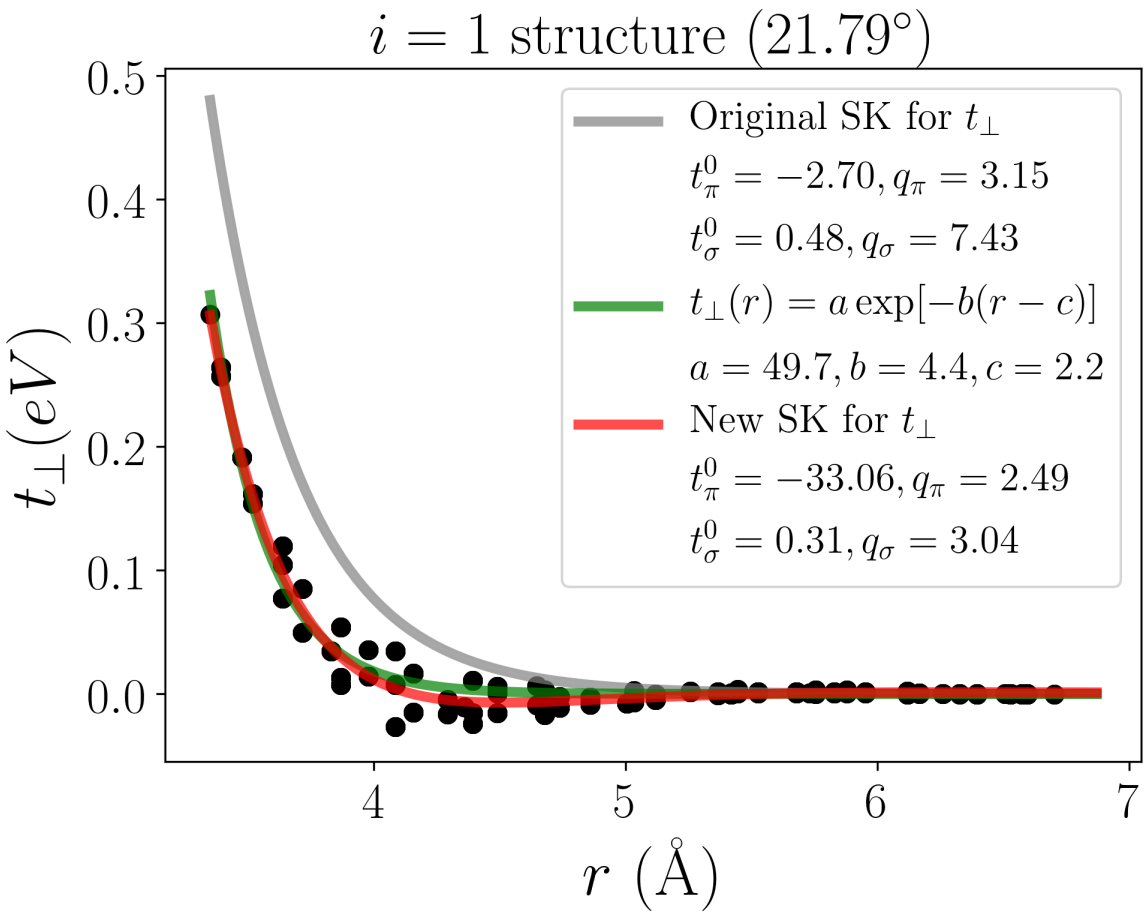
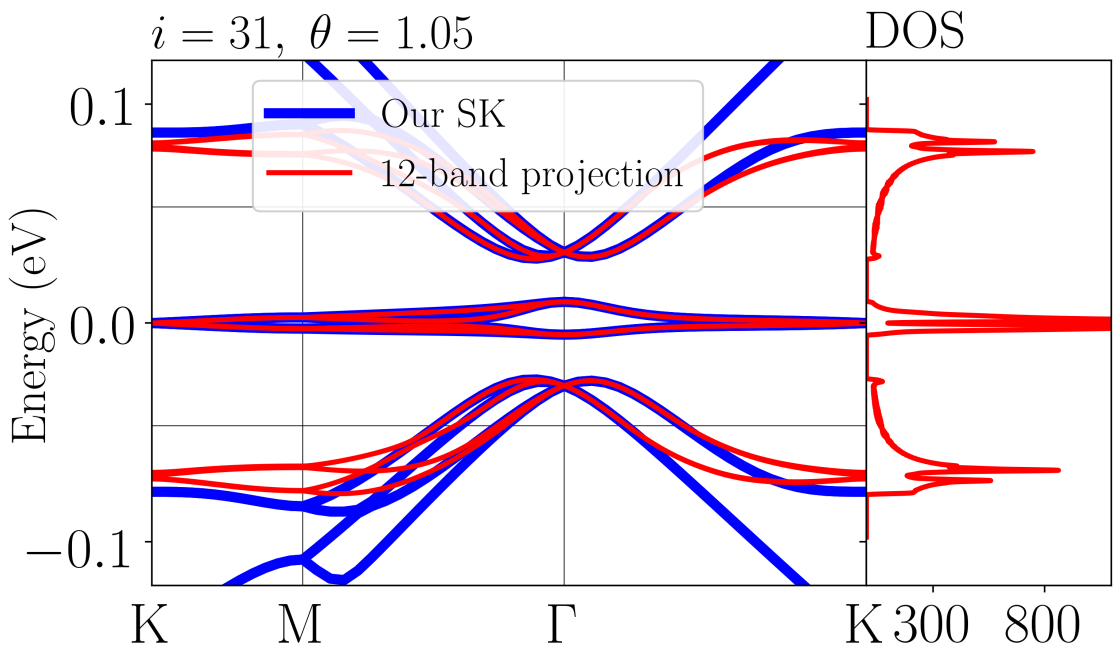
Wannierisation of DFT result

- Can we get a similar to SK parametrisation using *ab-initio* tight binding ?
- We follow the next path :
  (1) Fix in-plane hoppings ($t_{||}$) to ones for the SLG
  (2) Obtain all possible out-of-plane hoppings ($t_{\perp}$) from *ab-initio* calculations for large angles (21.79)
  (3) Construct an analytic function which reproduces (2) approximately as a function of distance (or other geometrical parameters)
  (4) Use this function to obtain $t_{\perp}$ for any smaller angles and plug it into a tight-binding Hamiltonian

$t_\perp(r)$ function



Bandstructure



Reducing Dimensions

- It is possible to reproduce the part of Hilbert space for low-energy Bloch states (blue lines) with further Wannierisation :

$$A_{mn\mathbf{k}} = \langle \psi_{m\mathbf{k}} | \tau_n \rangle$$

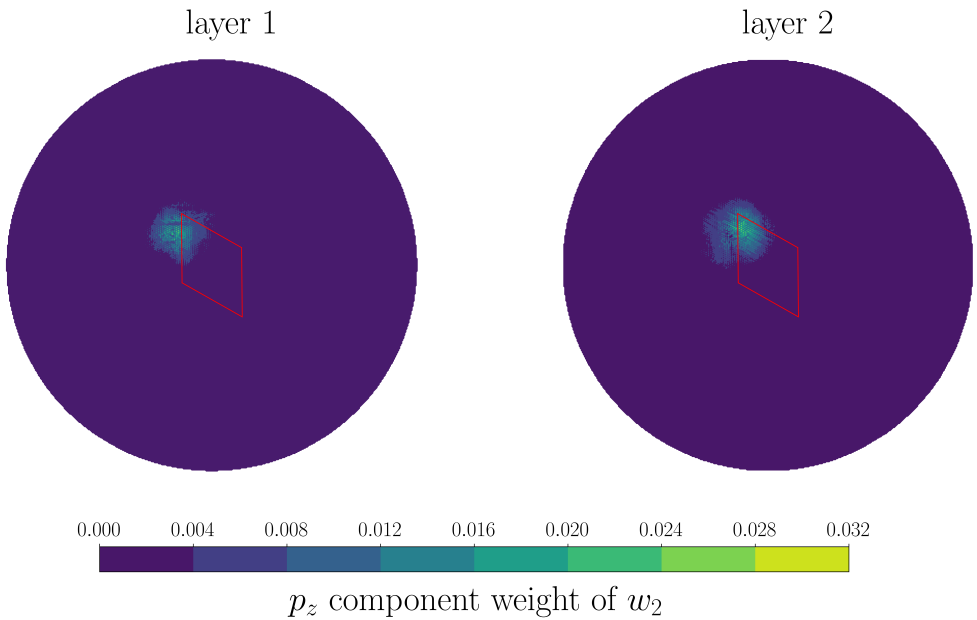
- This gives a basis $\varphi_n \leftarrow \psi_{m\mathbf{k}}$, and the old Hamiltonian in this new basis is :

$$t_{nm}(\mathbf{R}) = \langle \varphi_n(\mathbf{r}) | H(\mathbf{r}) | \varphi_m(\mathbf{r} - \mathbf{R}) \rangle$$

Final Wannier functions

- In principle we can trace back the real-space shape of Wannier orbitals
- But it is more practical to work with p_z-expansion :

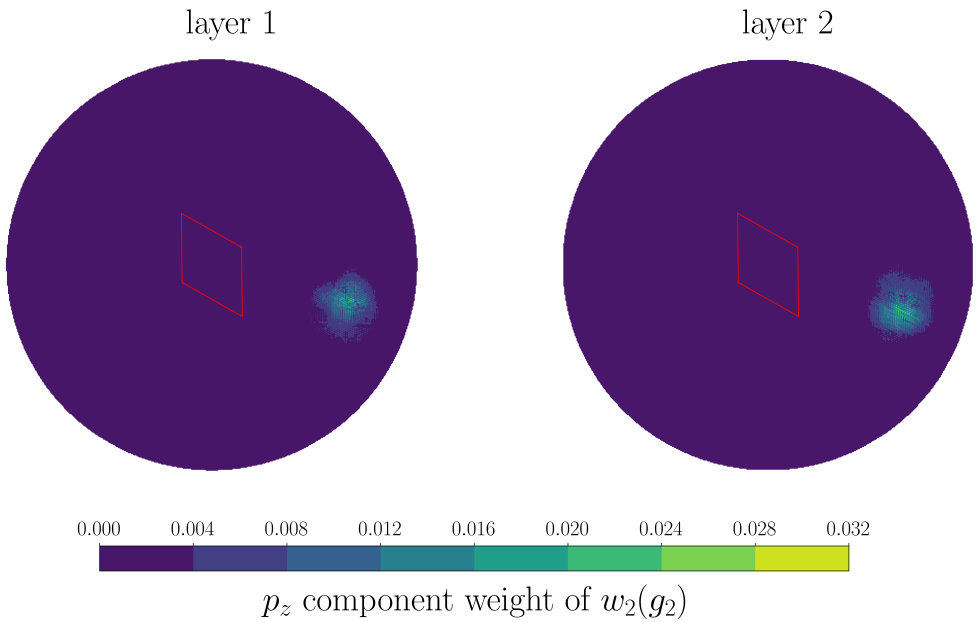
$$w(\mathbf{r}) = \sum_i C_i p_z(\mathbf{r} - \mathbf{r}_i), \mathbf{r}_i = \text{original C-atom position}$$



What about the symmetry ?

- In principle, we have symmetry operations in the real space, so we can :

$$gw(\mathbf{r}) = w(g^{-1}\mathbf{r}) \rightarrow C_{n \leftrightarrow m}$$



What about the symmetry ?

- Symmetry of Hamiltonian in a mathematical sense :

$$gH = D(g)HD(g^{-1})$$

- LA definition :

$$\begin{aligned} \tilde{w}_j &= \sum_i D_{ij} w_i \\ D_{ij} &= \langle w_i | g w_j \rangle \end{aligned}$$

- In principle, $\tilde{w}_j = g w_j$, and as a consequence :

$$\langle \tilde{w}_i | g w_j \rangle = \delta_{ij}$$

- However $\langle \tilde{w}_j | g w_j \rangle \to 0.9$ in my case

How to fix that ?

(1) Do the cycle transformation :

$$\tilde{w}_j^1 = \hat{D}(g_1^{-1}) g_1 w_j^0$$

(2) Construct the difference with original function :

$$\delta_j^1 = w_j^0 - \tilde{w}_j^1$$

(3) Extract the orthogonal projection onto δ_j^1 :

$$v_j^1 = w_j^0 - \langle \delta_j^1 | w_j^0 \rangle \delta_j^1$$

(4) do it for all symmetry operation consequently :

$$v_j^s = v_j^{s-1} - \langle \delta_j^s | v_j^{s-1} \rangle \delta_j^s$$

(5) go to (1) with $w_j^0 \leftarrow v_j^s$

Conclusion

(1) We made *ab-initio* calculation for larger angles (smaller UC) of TBG, to extract out-of plane hoppins

(2) Fit those to an analytic function $t_\perp(r, \vec{\alpha})$

(3) Solve the tight-binding Hamiltonian for an arbitrary angle using (2)

(4) Project the tight-binding Hamiltonian on a smaller basis set defined by the solutions of (3).

(5) Gerenrate symmmetrised Wannier basis from (4)

(6) Try to compute matrix elements of Hamiltonian directly on this symmetrised basis (next weeks project)

Symmetry representations p_z

- Our first TB model is written in "one p_z orbital per site" basis :

$$\psi(\mathbf{r}) = \sum_{i\mathbf{R}} C_{i\mathbf{R}} p_z(\mathbf{r} - \mathbf{r}_i - \mathbf{R})$$

- We know the p_z basis transformation for sure

$$g p_z(\mathbf{r} - \mathbf{r}_i - \mathbf{R}) = p_z(g^{-1}\{\mathbf{r} - \mathbf{r}_i - \mathbf{R}\})$$

- just to to know where centers transfrom :

$$D^{p_z}_{ij\mathbf{R}\mathbf{R}'}(g) = \left\langle p_z(\mathbf{r} - \mathbf{r}_i - \mathbf{R}) | g | p_z(\mathbf{r} - \mathbf{r}_j - \mathbf{R}') \right\rangle$$

D^{p_z} acts on coordintates $C_{i\mathbf{R}}$

Symmetry representations w_{nR}

- knowing D^{p_z}, we can construct symmetry representaion for wannier functions

$$\begin{aligned} D^{12}_{nn'\mathbf{R}\mathbf{R}'}(g) &= \langle w_{n\mathbf{R}}|g|w_{n'\mathbf{R}'}\rangle \\ &= \langle w_{n\mathbf{R}}|D^{p_z}(g)|w_{n'\mathbf{R}'}\rangle \\ &= \sum_{ij\mathbf{T}\mathbf{T}'} \left\langle w_{n\mathbf{R}}(\mathbf{T}+\mathbf{r}_i) \left| D^{p_z}_{ij\mathbf{T}\mathbf{T}'}(g) \right| w_{n'\mathbf{R}'}(\mathbf{T}'+\mathbf{r}_j) \right\rangle \end{aligned}$$

Partial density of states