ETH zürich

Spectral properties of hybrid bilayer graphene

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Motivation and strategy

- Flat band superconductivity in experimentally tunable systems, using superstructures of weakly correlated 2D materials

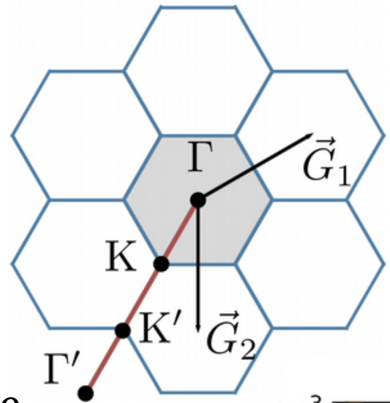
- Experimental tools
  $\longrightarrow$ twist angle (Bistritzer & MacDonald, PNAS2011)
  $\longrightarrow$ atomic defects (Lopez-Bezanilla PRM2019, Ramires PRB2019)

- Compare physics of superlattices: defects vs. moiré

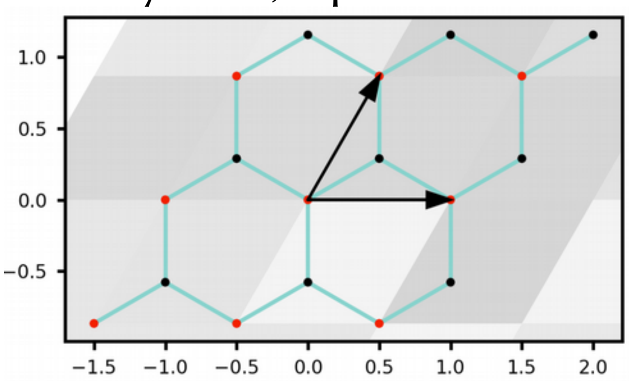
- Enhance DOS in order to suppress the kinetic term
  $\longrightarrow$ possibly high correlations $\longrightarrow$ unconventional SC

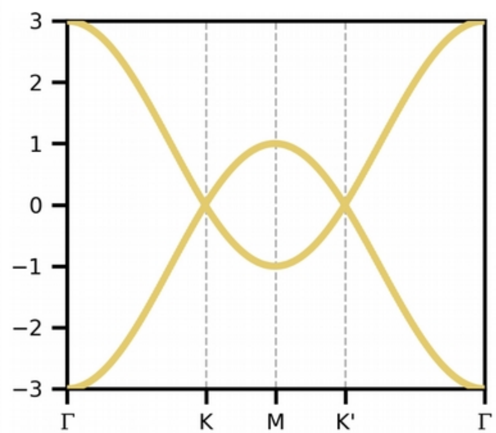
Graphene

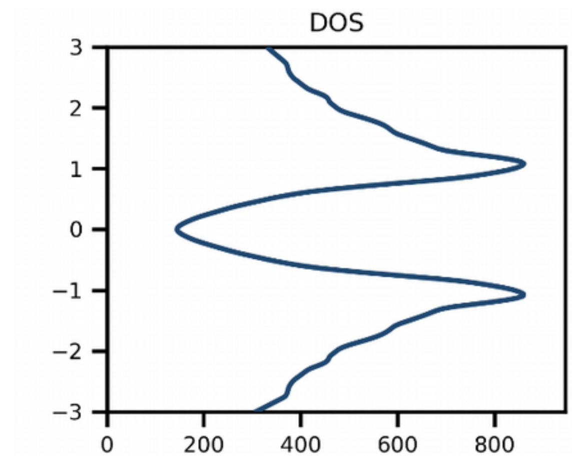
$$H = \sum_{\langle i,j \rangle} t c_i^\dagger c_j$$



Honeycomb, bipartite







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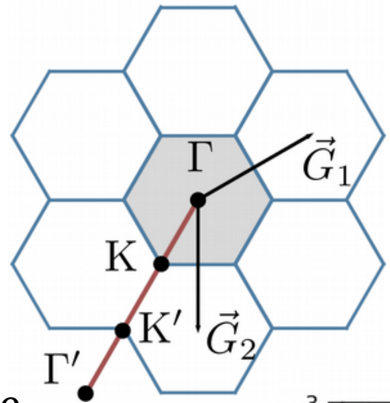
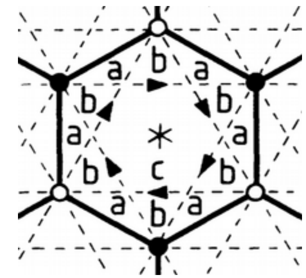


Valley flavour $\eta_{ij} = \pm$

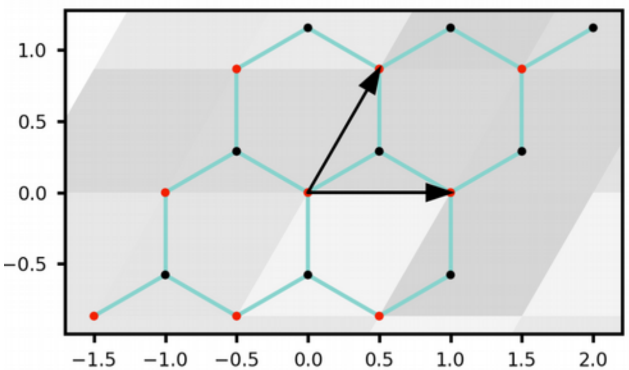
$$H_{\mathrm{aH}} = \frac{i}{3\sqrt{3}} \sum_{\langle\langle i,j \rangle\rangle} \eta_{ij} \sigma_z^{ij} c_i^\dagger c_j$$

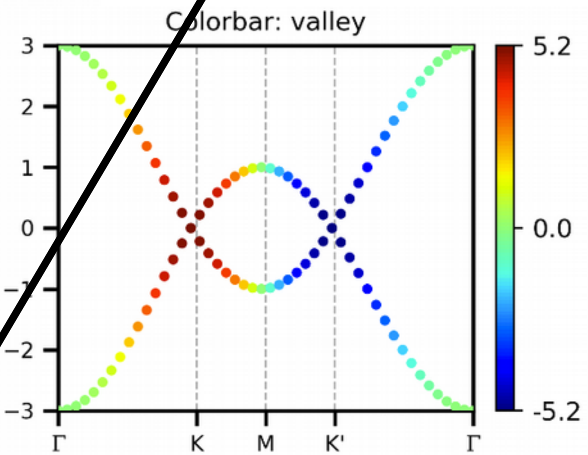
Ramires PRB2019

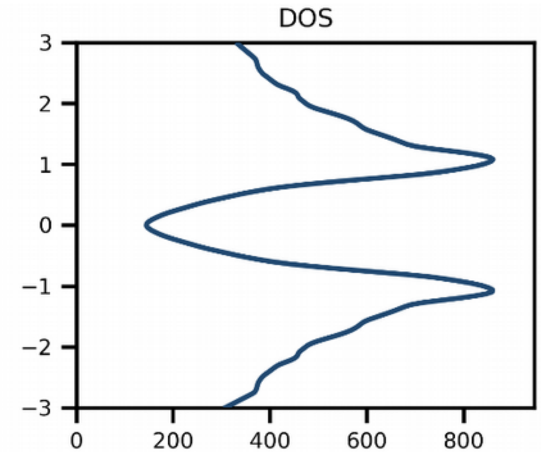


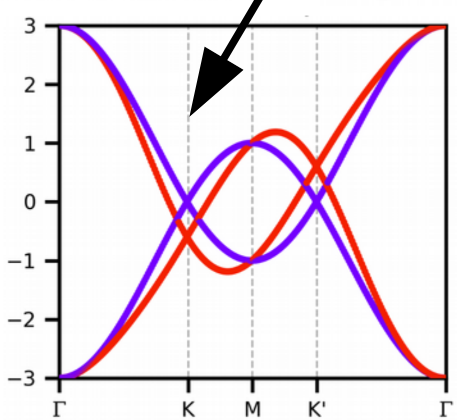
Haldane PRL1998

Honeycomb, bipartite









The "Anti-Haldane" hopping term shifts the energy of the Dirac points at K and K' in opposite directions

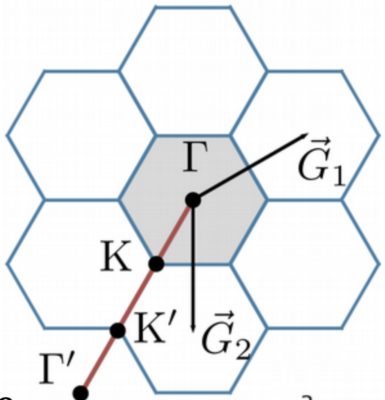
$\longrightarrow$ purple: H

$\longrightarrow$ red: $H + H_{\mathrm{aH}}$

Use it as projection operator: color $= \langle \psi | H_{\mathrm{aH}} | \psi \rangle$

Graphene

$$H = \sum_{\langle i,j \rangle} t c_i^\dagger c_j$$



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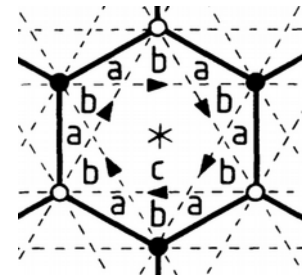
Ramires PRB2019



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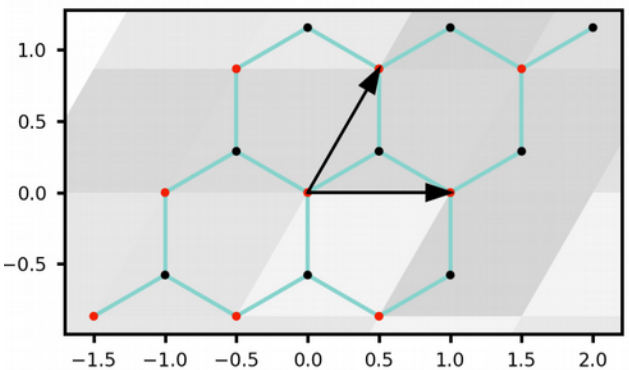
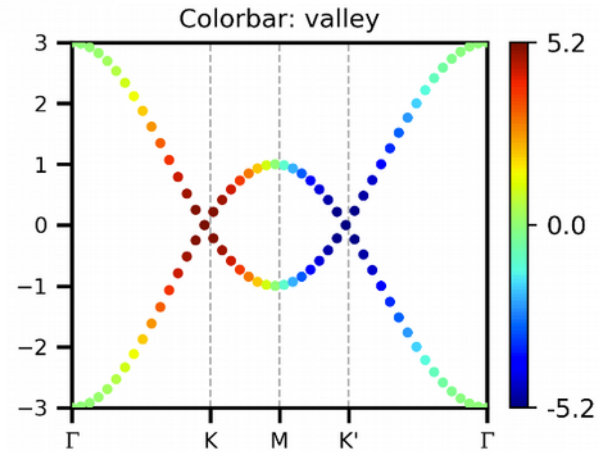
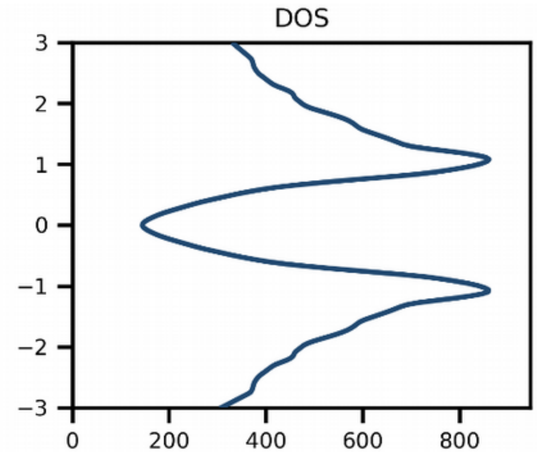
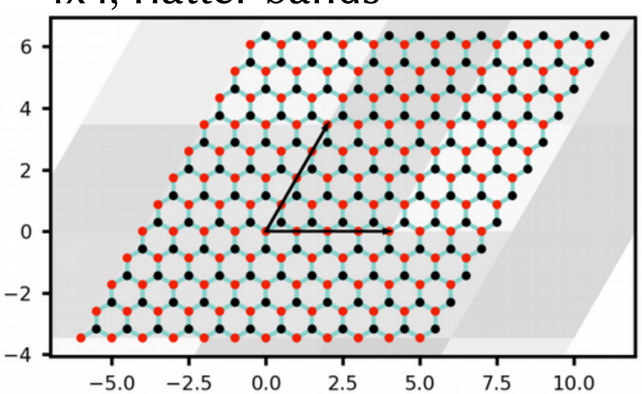
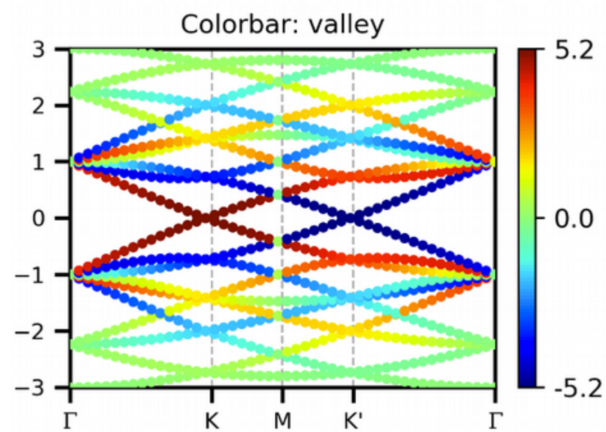


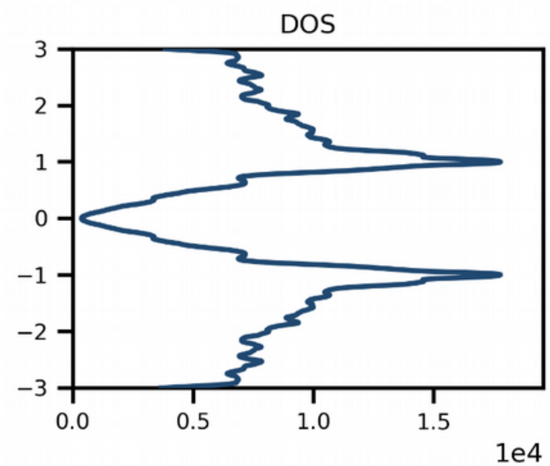




4x4, flatter bands

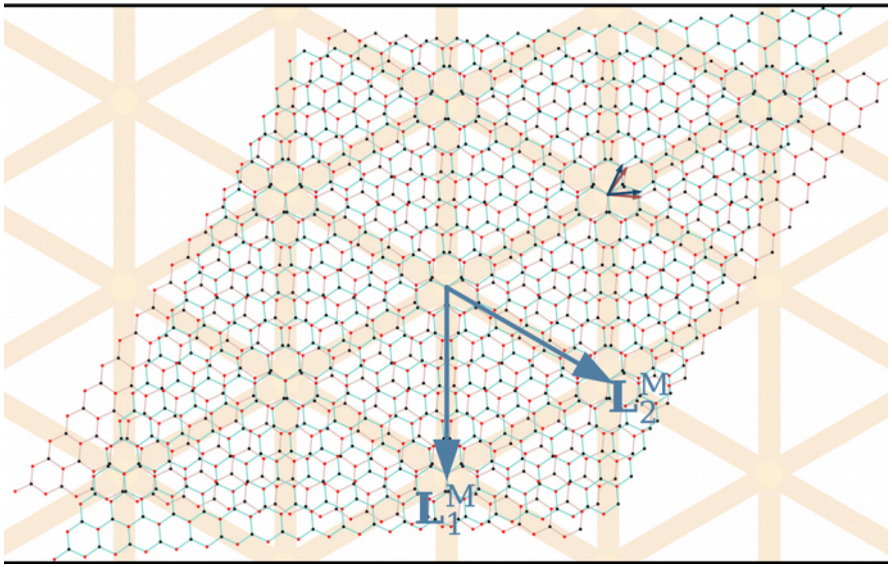




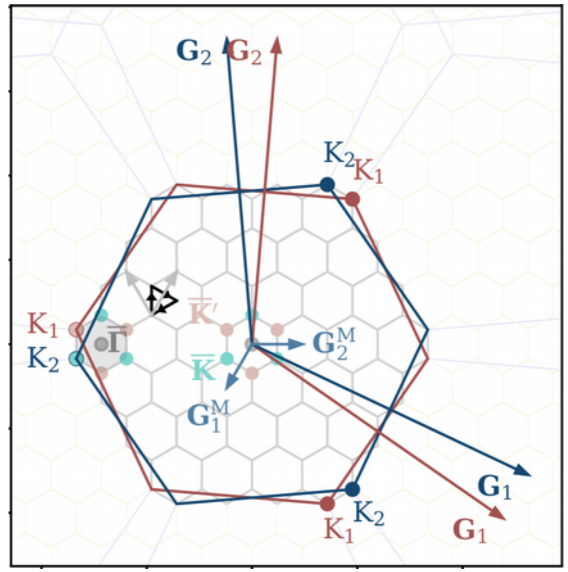


Moiré pattern and van Hove singularities

small relative twist ⟶ moiré superlattice



Certain angles: periodic



r=1

$$\cos\theta(m,r) = \frac{3m^2+3mr+r^2/2}{3m^2+3mr+r^2}$$

$$\begin{bmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \end{bmatrix} = \begin{bmatrix} m & m+r \\ -(m+r) & 2m+r \end{bmatrix} \begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \end{bmatrix}$$

Neto PRB2012

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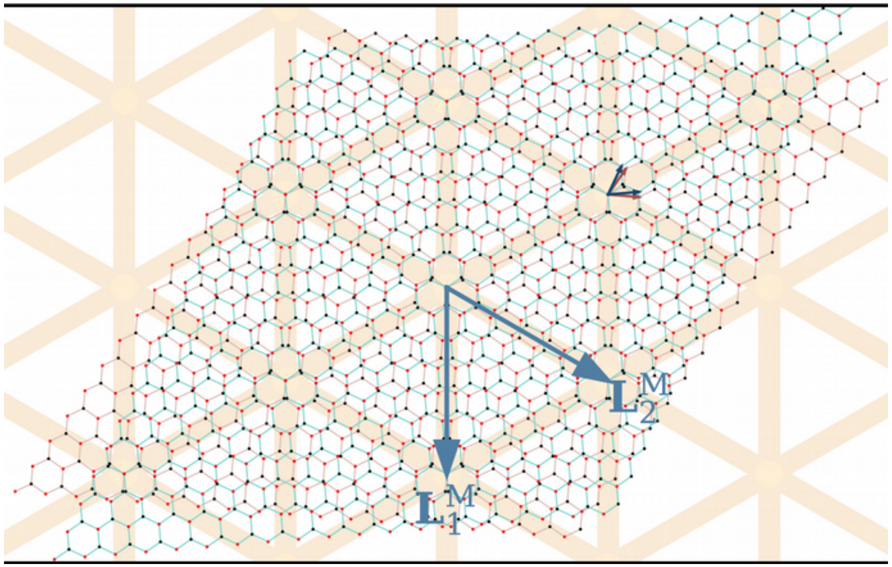

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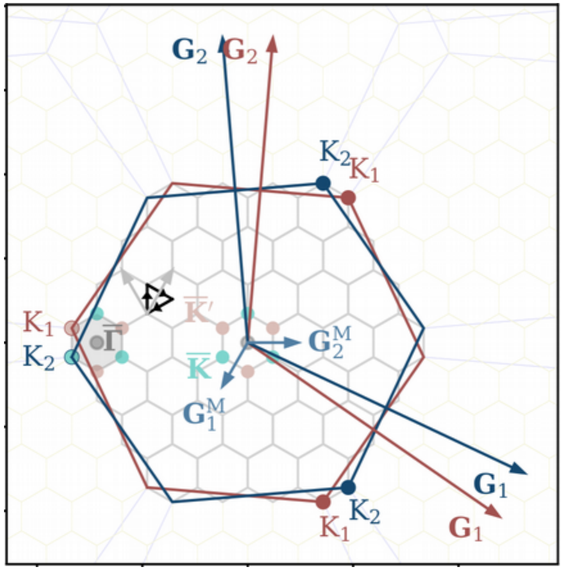
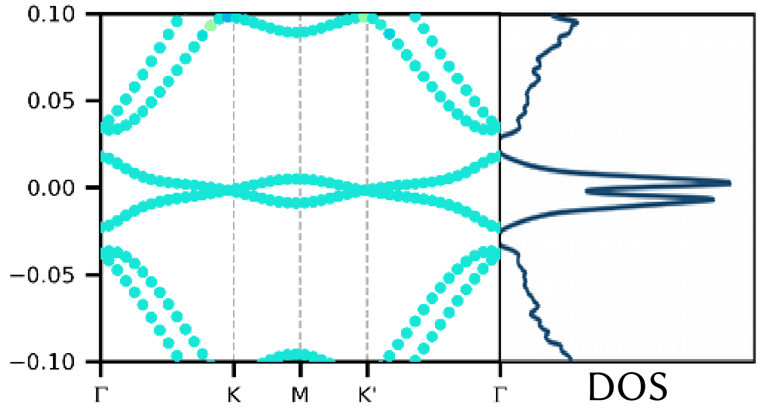


BZ folding flattens the bands at low energy



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Neto PRB2012

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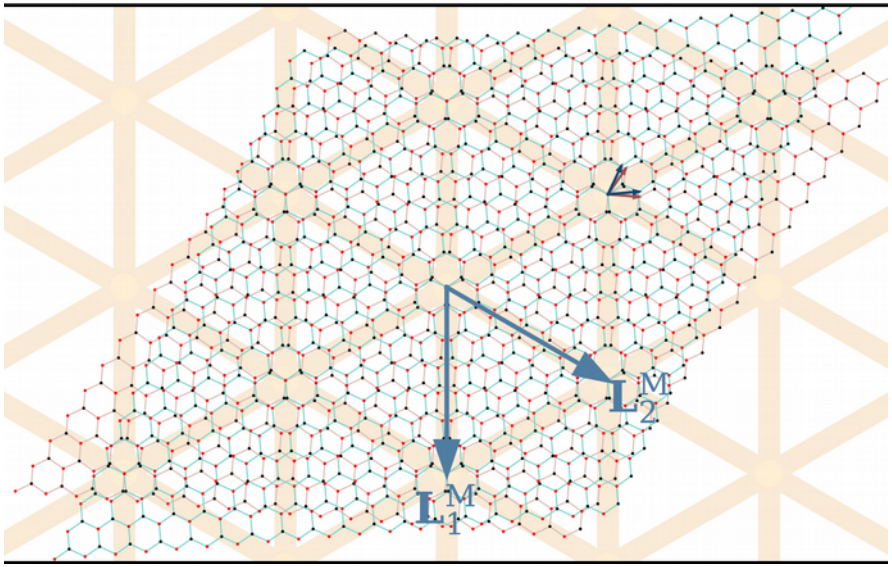
small relative twist → moiré superlattice



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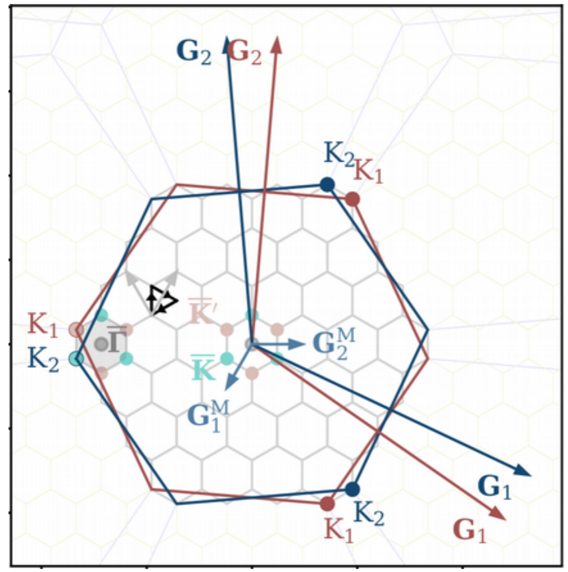

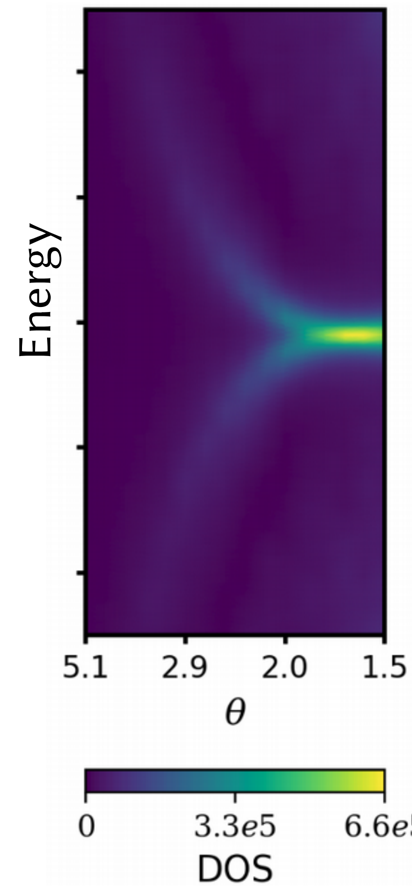

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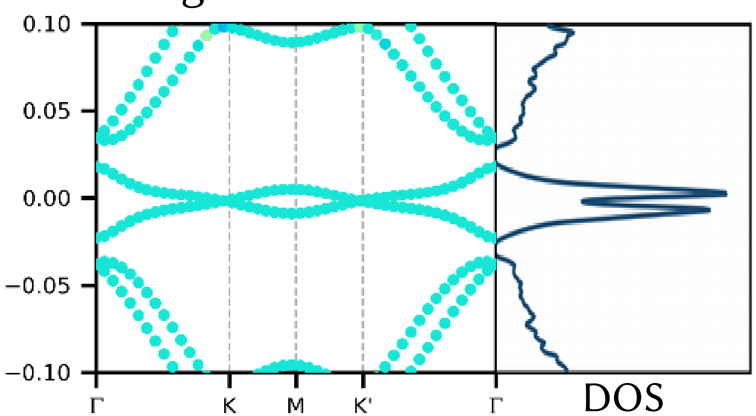

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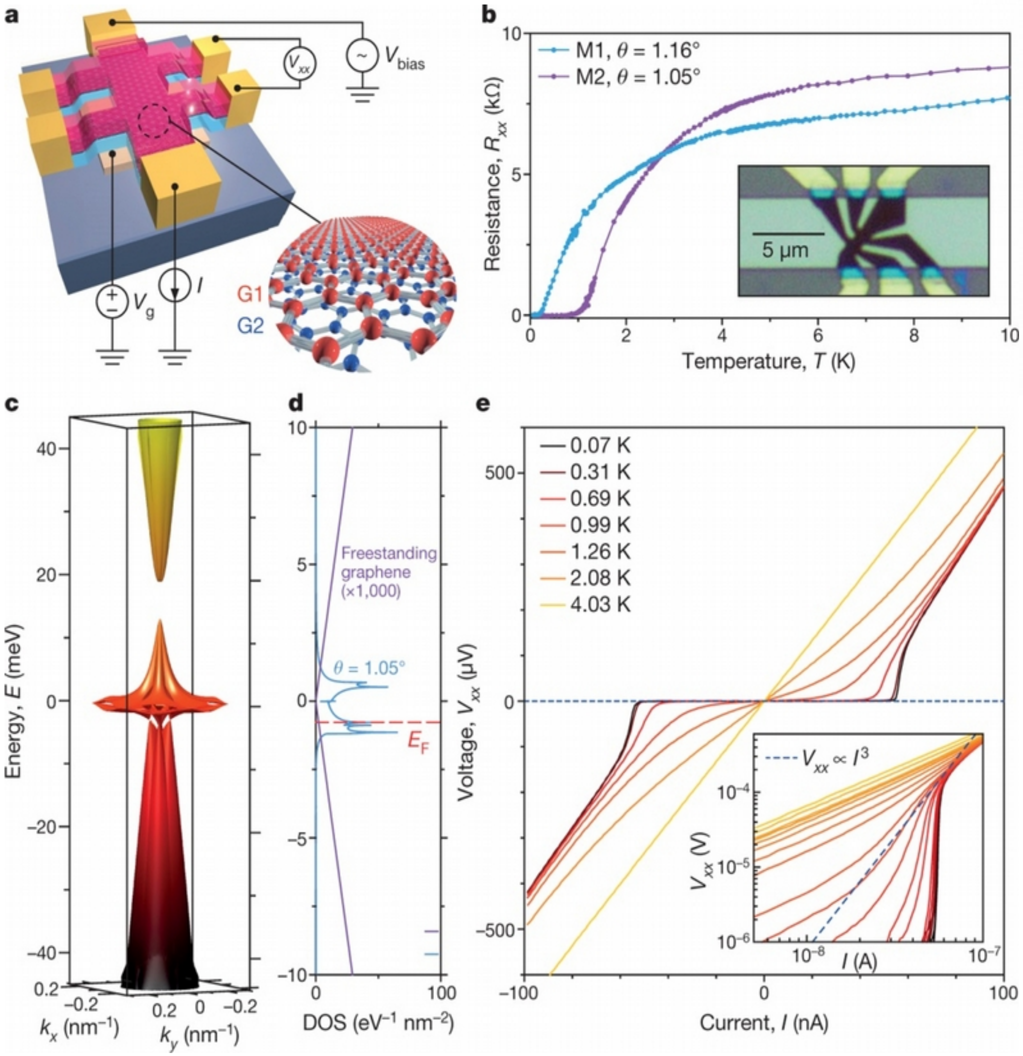
Neto PRB2012

Superconductivity in TBG



Superfluidity in system with fermion condensate

V. A. Khodel' and V. R. Shaginyan
I. V. Kurchatov Institute of Atomic Energy, Moscow; B. P. Konstantinov Institute of Nuclear Physics, Academy of Sciences of the USSR

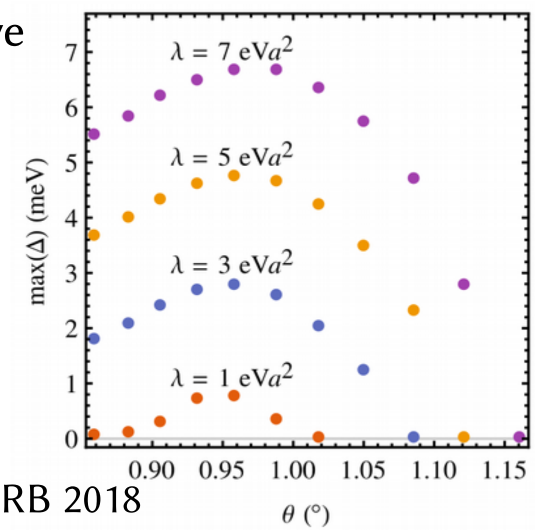
(Submitted 4 April 1990)
Pis'ma Zh. Eksp. Teor. Fiz. **51**, No. 9, 488–490 (10 May 1990)

The properties of Fermi systems beyond the phase transition point, at which the group velocity of the quasiparticles changes sign on the Fermi surface, are analyzed. A Fermi condensate arises in the new phase: The energies $\epsilon(\mathbf{p})$ of quasiparticles with momenta $p_{1c} < p < p_{2c}$ $(p_{1c} < p_F, p_{2c} > p_F)$ turn out to be identical and equal to the chemical potential μ. If a Cooper pairing can occur in this phase the gap Δ is a linear function of the pairing constant λ.

BCS: $\Delta \propto e^{-1/\mathcal{D}(0)\lambda}$

Inside van Hove singularity:

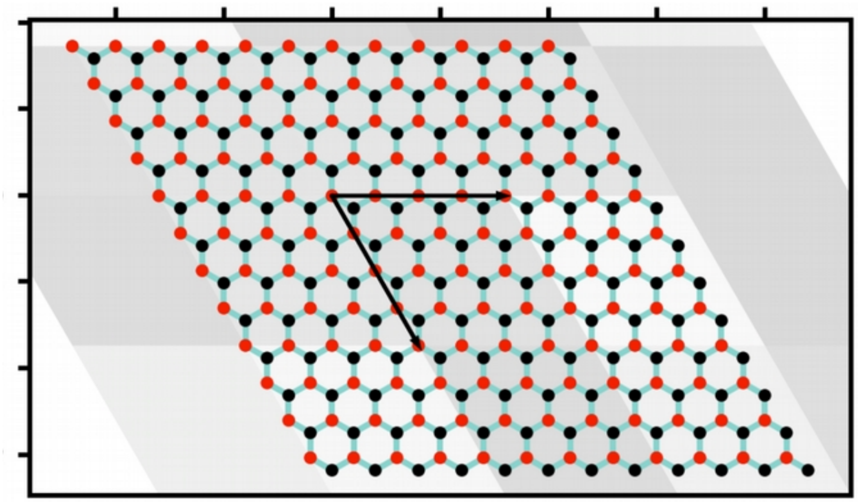
$\Delta \propto \lambda$



Peltonen PRB 2018

nature Cao 2018

Other mechanism which flattens the low-energy bands



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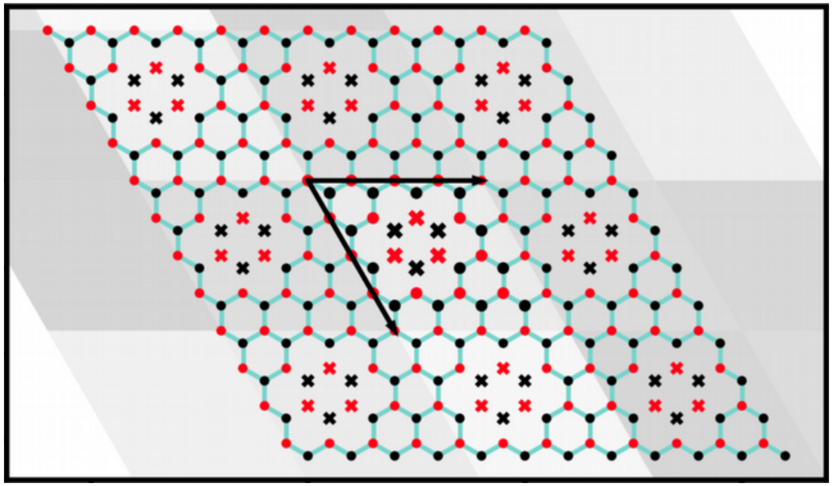
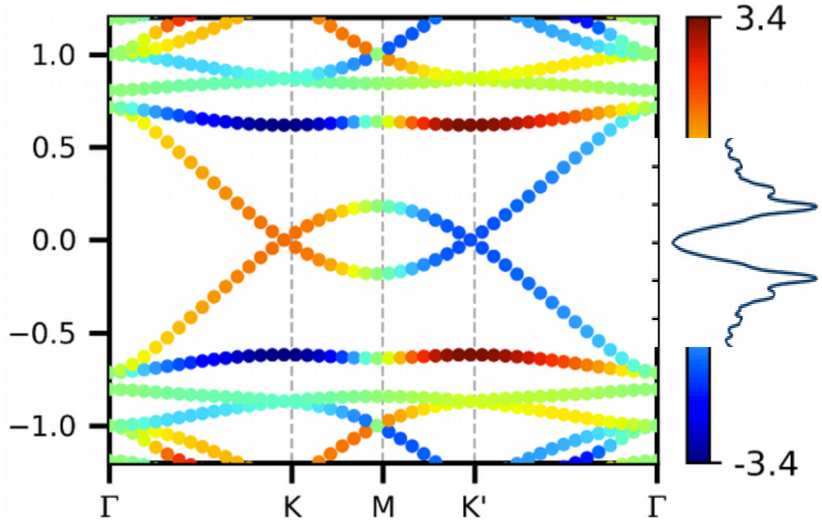
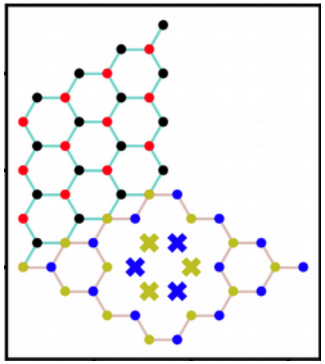




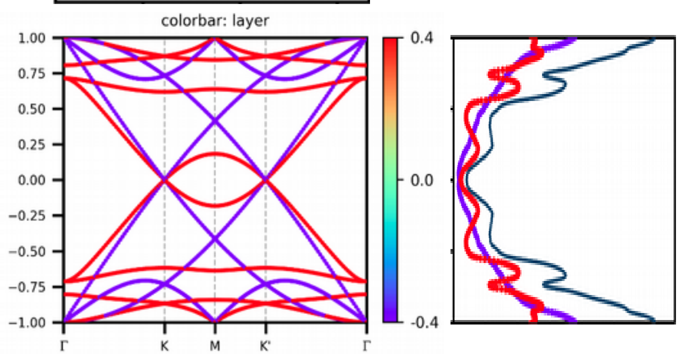
- The UC has 4x4x2-6=28 atoms
- The position of the removed hexagon in the UC is irrelevant

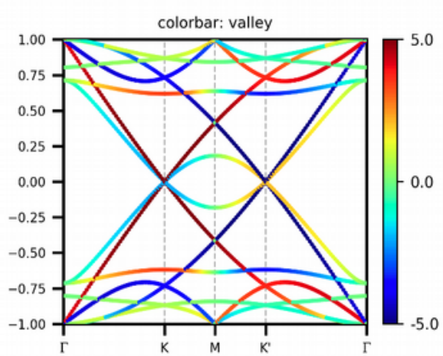
- Low-energy ~ graphene spectrum
  - Renormalized t
  - Weaker valley polarization
- Combined with a pristine layer ?

Hybrid TBG



4x4, 60deg
No coupling





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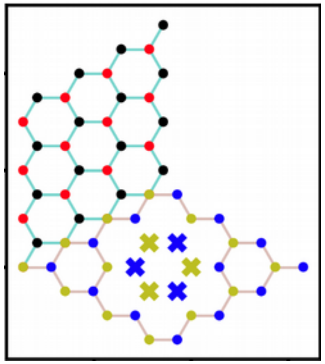

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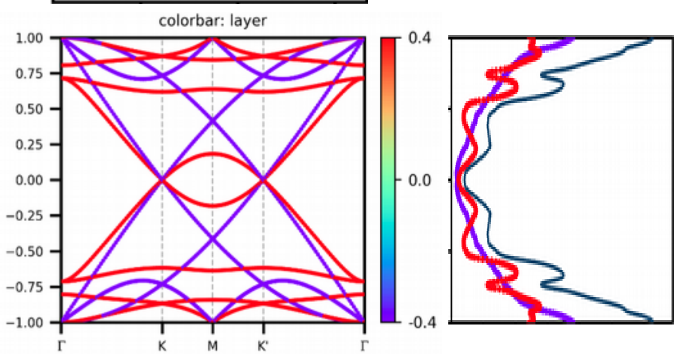
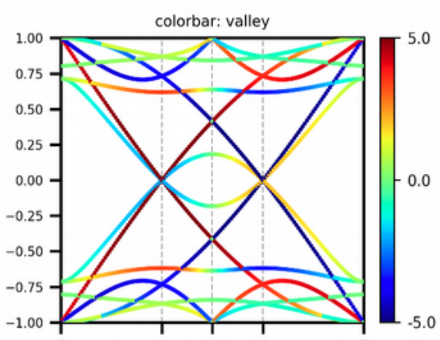
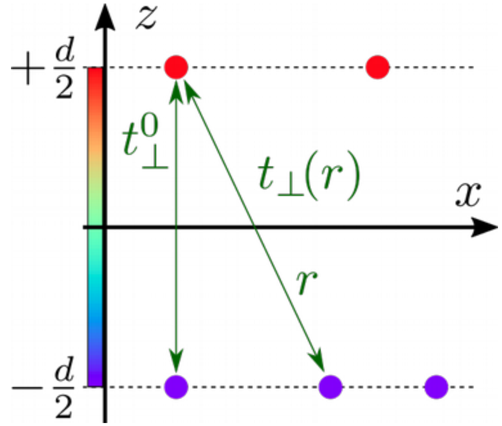






$$H_{\text{inter}} = \sum_{i\uparrow,\, j\downarrow} t_\perp(\mathbf{r}_i - \mathbf{r}_j) c_i^\dagger c_j + \text{H.c.}$$

$$t_\perp(\mathbf{r}) = t_\perp^0 \frac{z^2}{r^2} e^{-(r-d)/l}$$

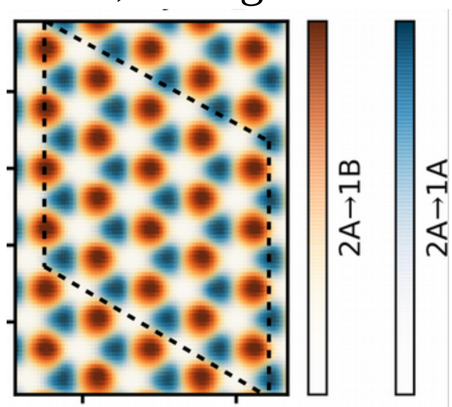
Sboychakov PRB2015
≈ only σ bonds

$t_\perp^0 = 0.25t \qquad d = 1.4a \quad l = 0.1a$

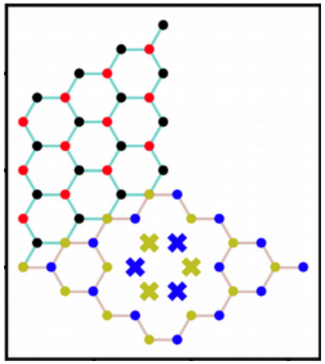
(2x larger, angle 2x smaller)

Gonzalez-Arraga, PRL2017

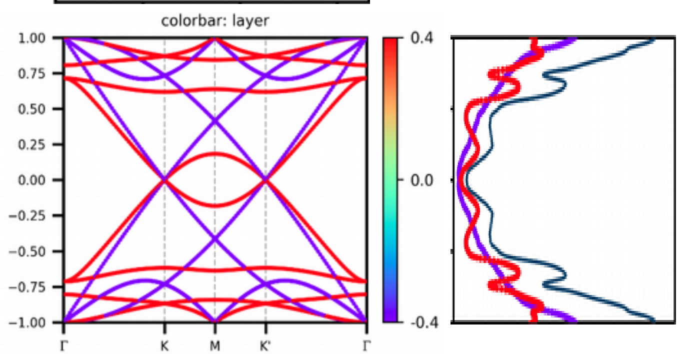
4x4, 7.3deg

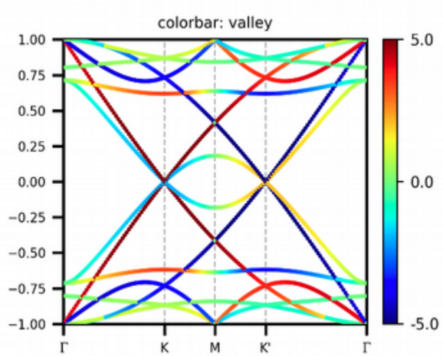


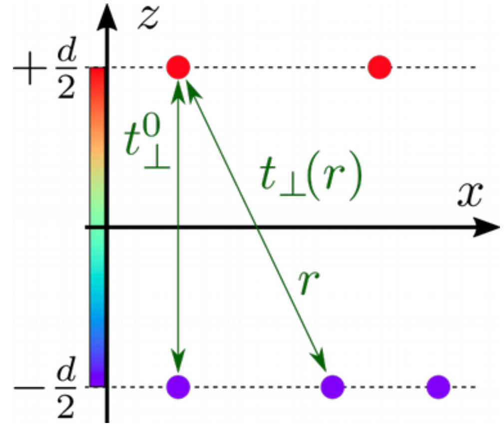
Hybrid TBG



4x4, 60deg
No coupling







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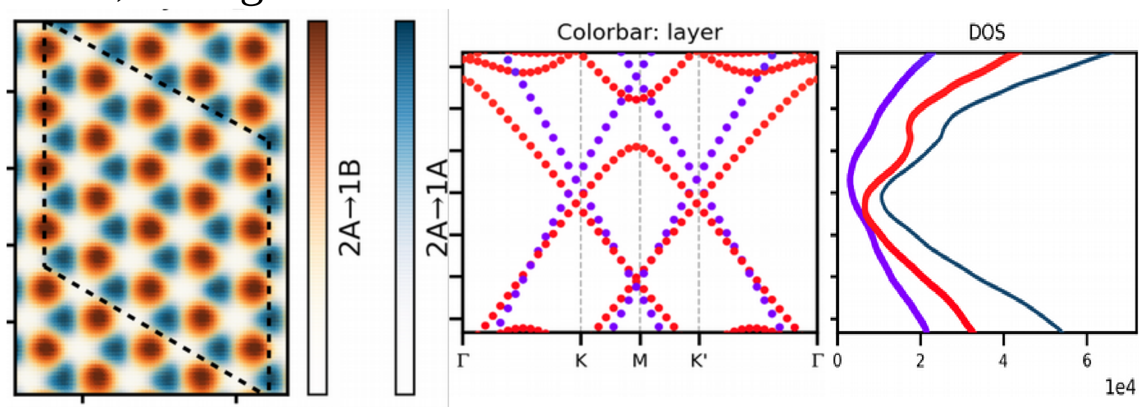
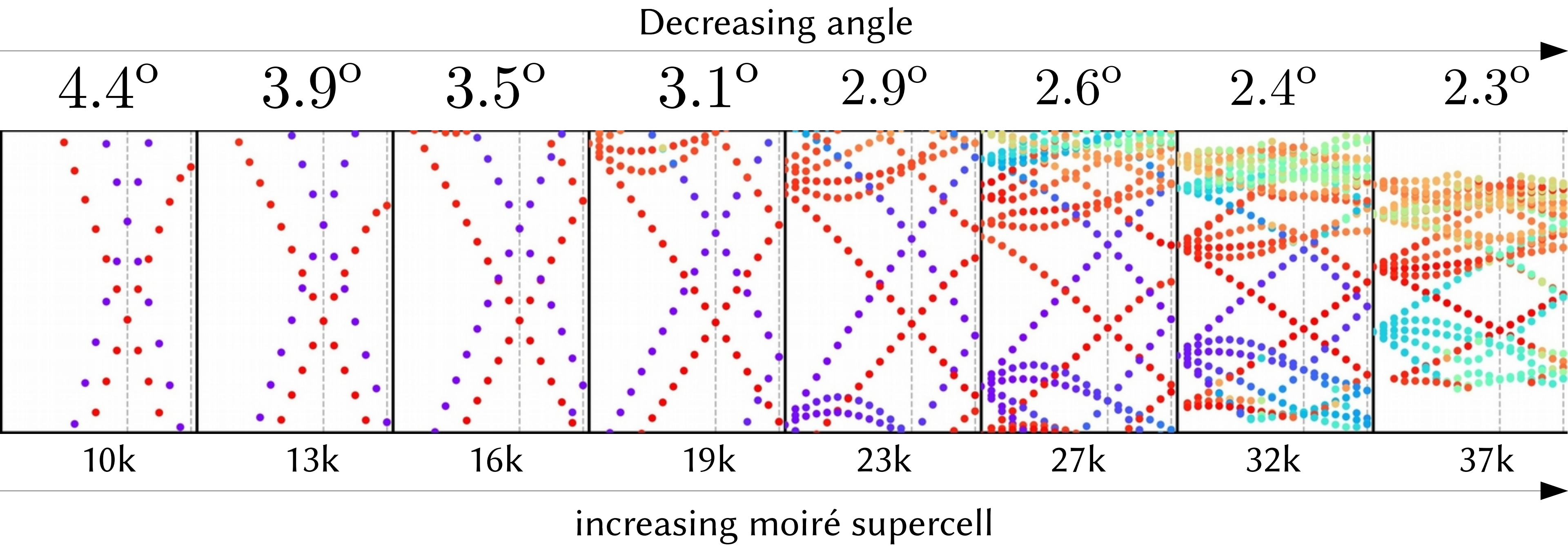


→ The En of the states in the upper layer is shifted down
→ Their Fermi velocity is reduced
→ Intervalley scattering only in the upper layer

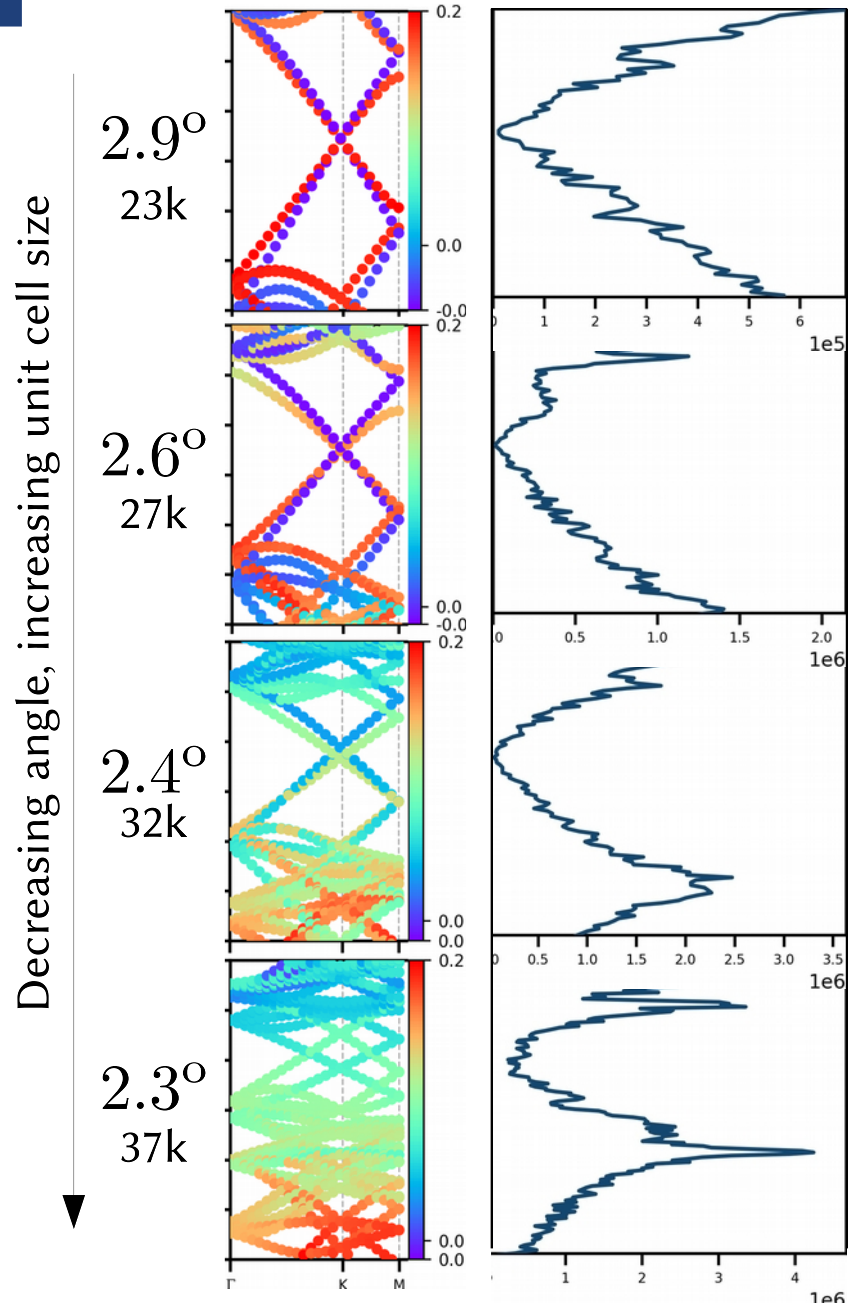
Small-angle hybrid TBG



The Energy difference between the cones is almost constant

$\longrightarrow$ related to the coupling strength and the vacancy concentration

$\longrightarrow$ the degeneracy of the cones can be restored using an electric field



Degenerate cones?

$$H = t_{\uparrow} \sum_{\langle i,j\rangle \in \uparrow} c_i^{\dagger} c_j \; + t_{\downarrow} \sum_{\langle i,j\rangle \in \downarrow} c_i^{\dagger} c_j$$

$$+ \sum_{i\in\uparrow,\; j\in\downarrow} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j) c_i^{\dagger} c_j$$

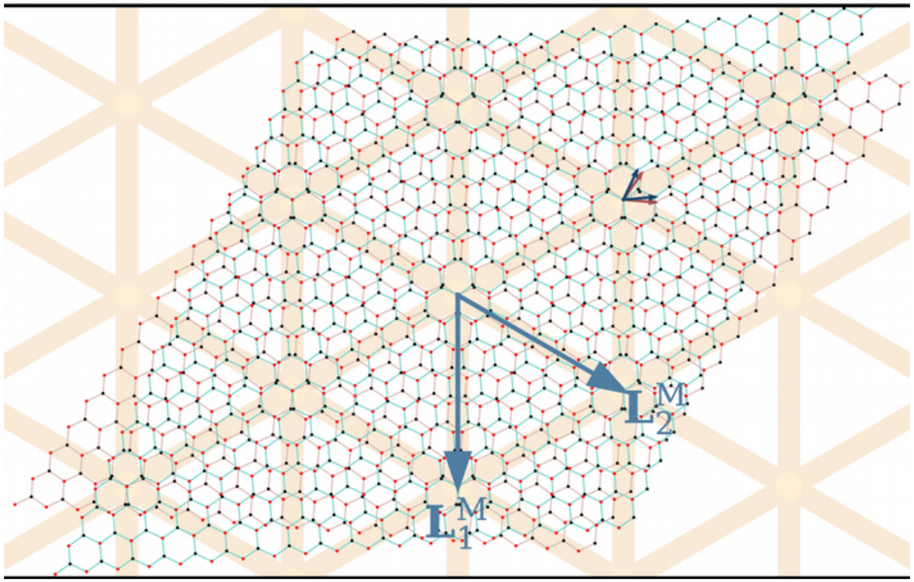
$$+ E \sum_{i\in\{\uparrow,\downarrow\}} z_i c_i^{\dagger} c_i$$

- Apply electric field E to restore the degeneracy of the Dirac points

- The states tend to localize in the upper layer as the interlayer coupling becomes stronger

- At small angles the Electric field is innefective because of the weak layer polarization.

Toy model



2 honeycomb layers, no vacancies

→ Displacement of the two pairs of Dirac cones using an electric field
→ Reduced Fermi velocity using a smaller t in the upper layer

Intra-layer hoppings | Inter-layer hopping | Electric field

$$H = t_\uparrow \sum_{\langle i,j\rangle \in \uparrow} c_i^\dagger c_j + t_\downarrow \sum_{\langle i,j\rangle \in \downarrow} c_i^\dagger c_j + \sum_{i\in\uparrow,\, j\in\downarrow} t_\perp(\mathbf{r}_i - \mathbf{r}_j) c_i^\dagger c_j + E \sum_{i\in\{\uparrow,\downarrow\}} z_i c_i^\dagger c_i$$

$t_\uparrow < t$

$t_\uparrow = t$

Bottom layer: pristine graphene

Toy model: spectra

$$H = t_{\uparrow} \sum_{\langle i,j \rangle \in \uparrow} c_i^\dagger c_j \; + \; t_{\downarrow} \sum_{\langle i,j \rangle \in \downarrow} c_i^\dagger c_j \; + \sum_{i \in \uparrow,\, j \in \downarrow} t_{\perp}(\mathbf{r}_i - \mathbf{r}_j) c_i^\dagger c_j + E \sum_{i \in \{\uparrow,\downarrow\}} z_i c_i^\dagger c_i$$

$t_{\uparrow} = 0.65t$

$t_{\uparrow} = t$

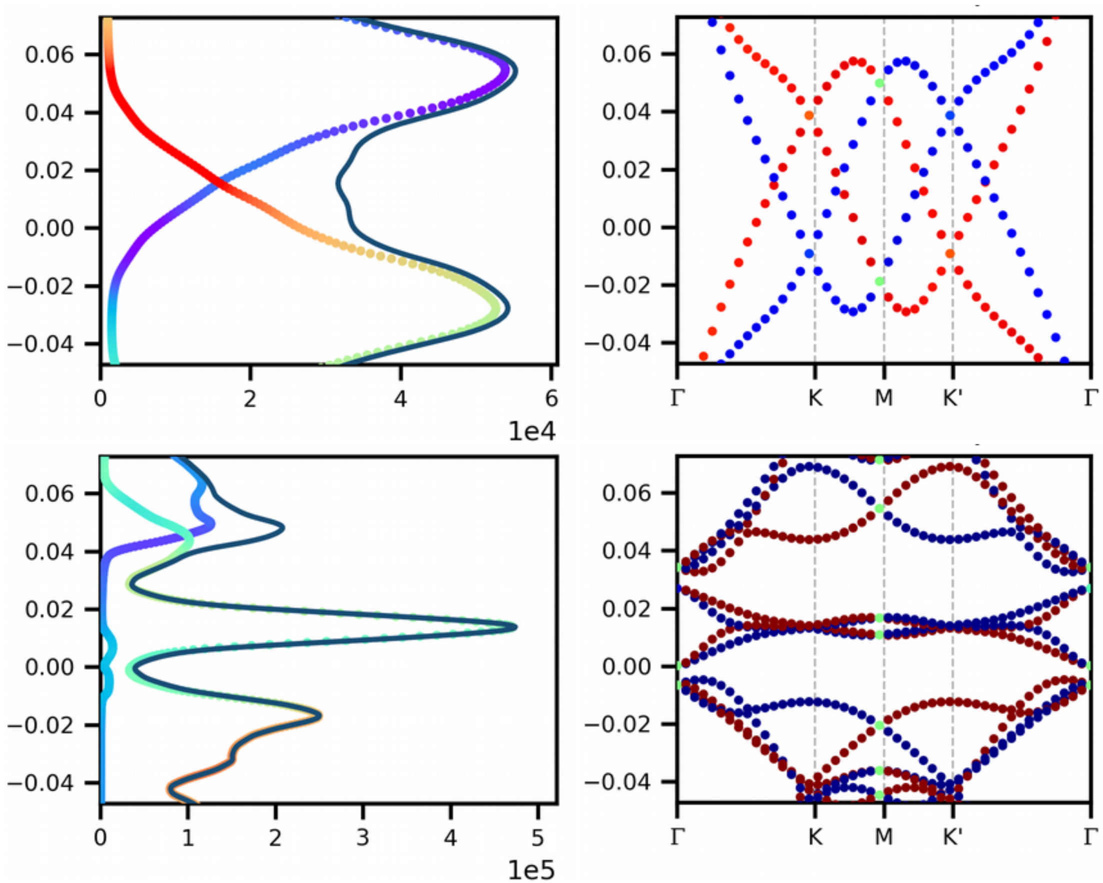
$E = 0.19t$

DOS per layer & total

Bands, valley flavour

4.4 deg

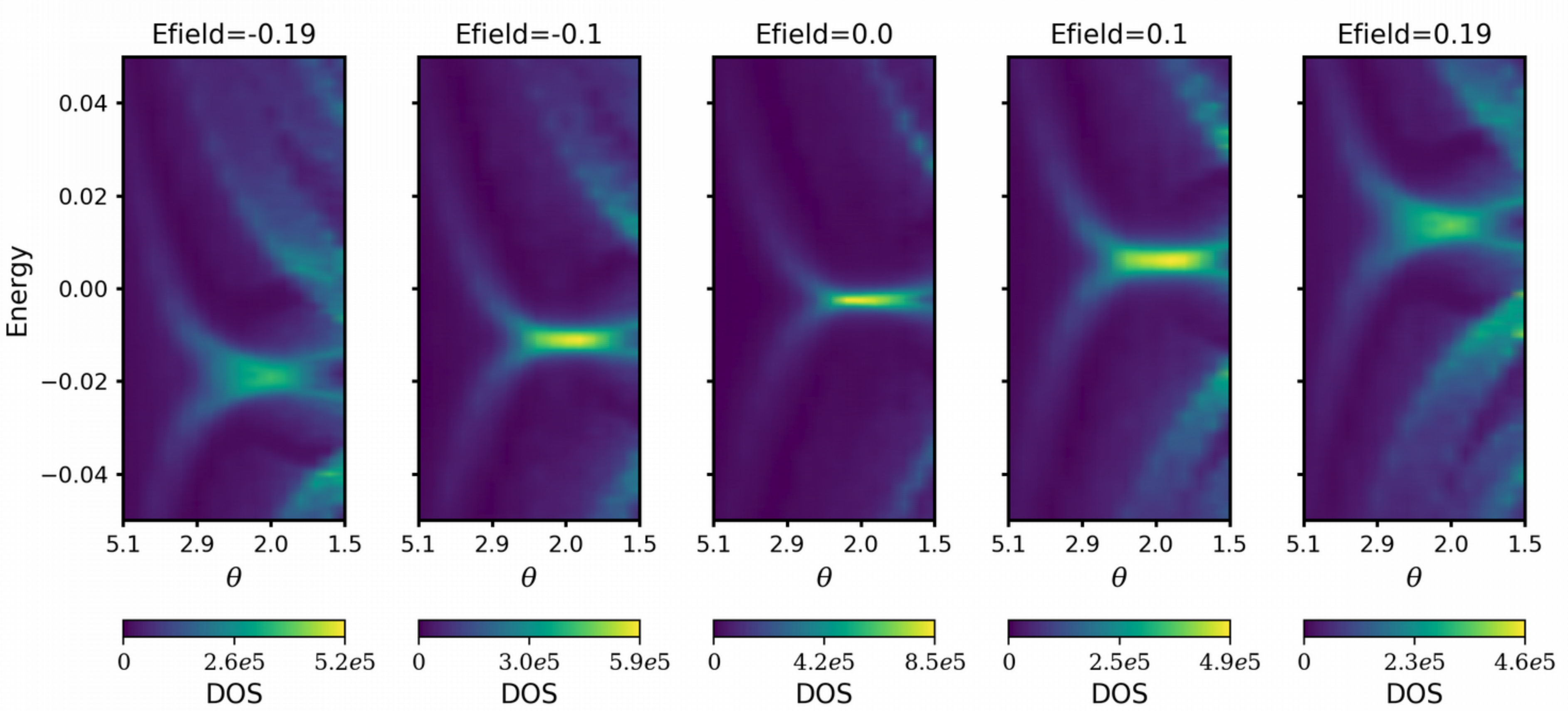
2.0 deg



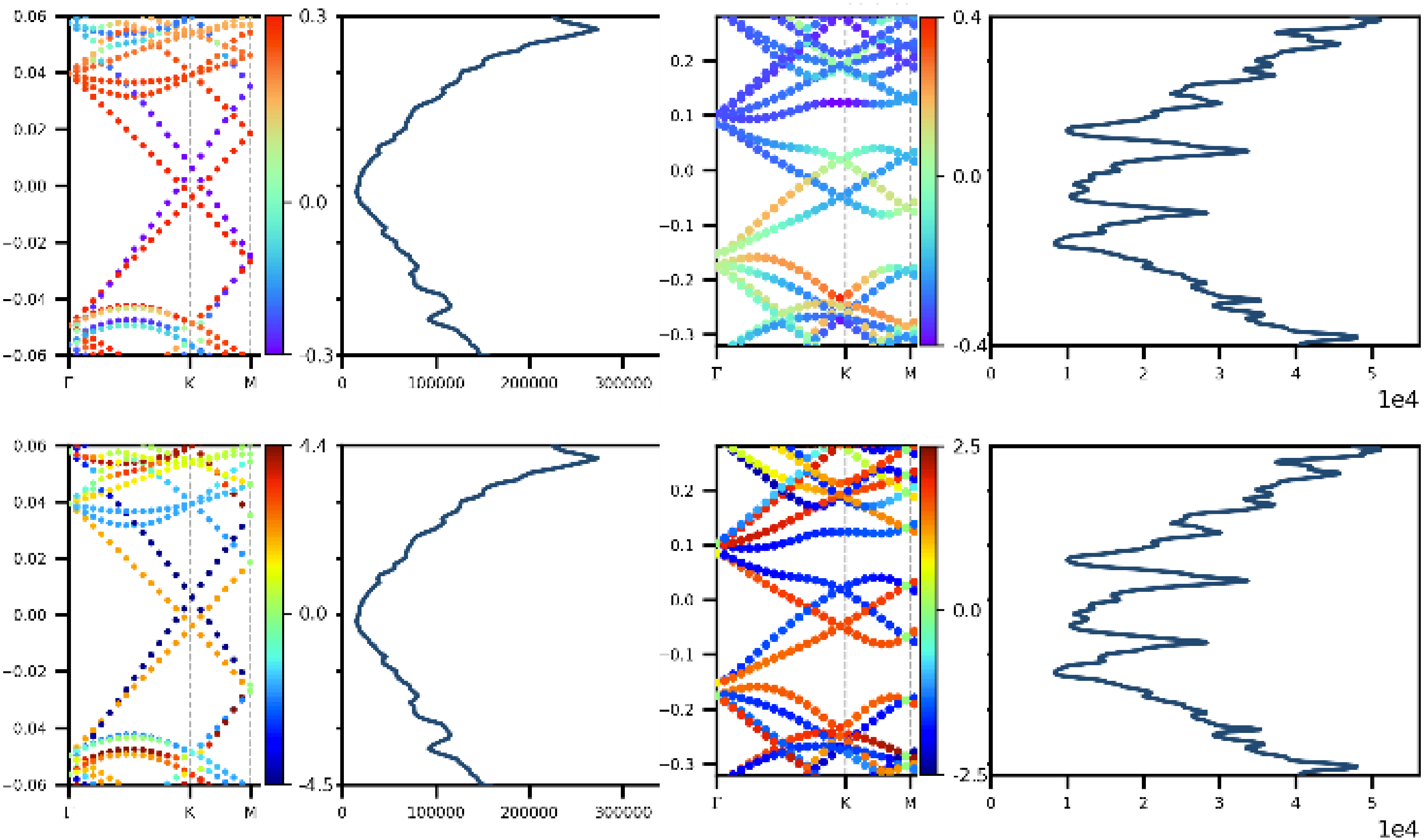
E acts like a valley-dependent anti-Haldane term.

Larger magic angle(s)

Toy model: DOS vs angle



Yet to understand: hybrid bilayer vs. toy model



Thank you for your attention!