Accuracy of a moiré Wannier function model for twisted bilayer graphene

Anushree Datta
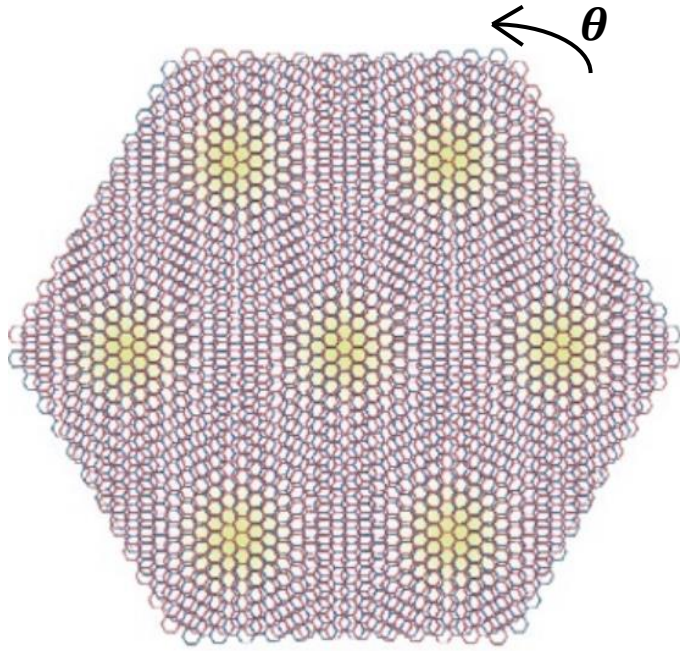
[Instituto de Ciencia de Materiales de Madrid (ICMM)-CSIC, Spain]
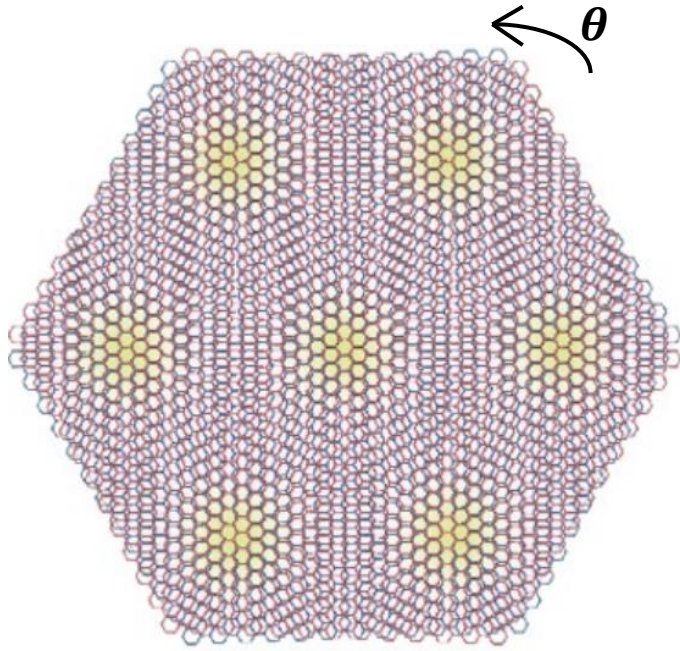
In collaboration with:

**María José Calderón (ICMM-CSIC),
Elena Bascones (ICMM-CSIC)**

Capri Spring School

iCMM CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

θ

θ

Continuum model

Bistritzer and Macdonald,
PNAS 108, 12233 (2011)

θ

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**Atomistic model
(~10^4 carbon atoms
per unit cell at small
twist angles)**
Moon and Koshino
PRB 85, 195458 (2012)

Moiré superlattice

θ

$L_M \sim 13\ nm$ for
$\theta = 1.1^0$
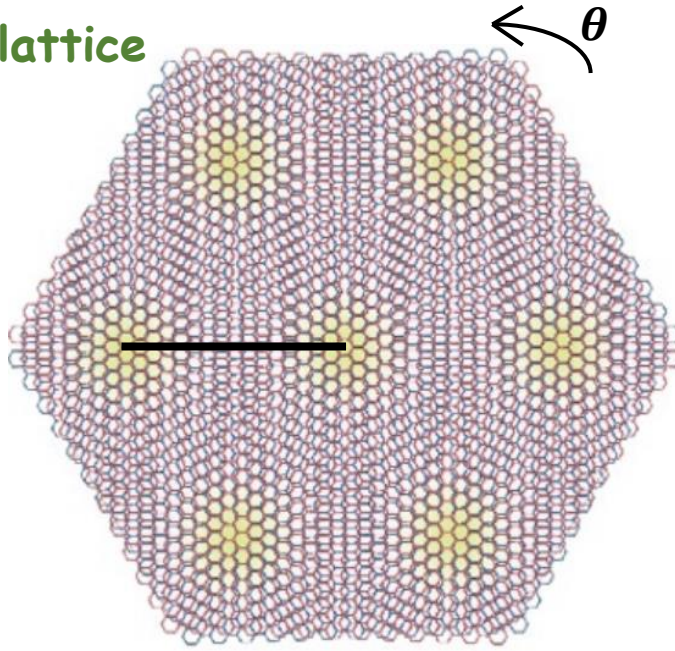

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**Model with effective
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Koshino et al., PRX 8, 031087 (2018)

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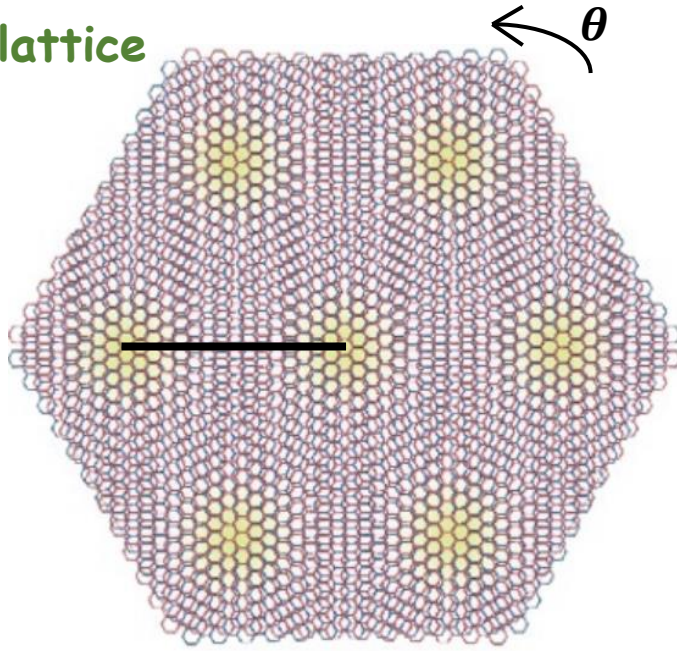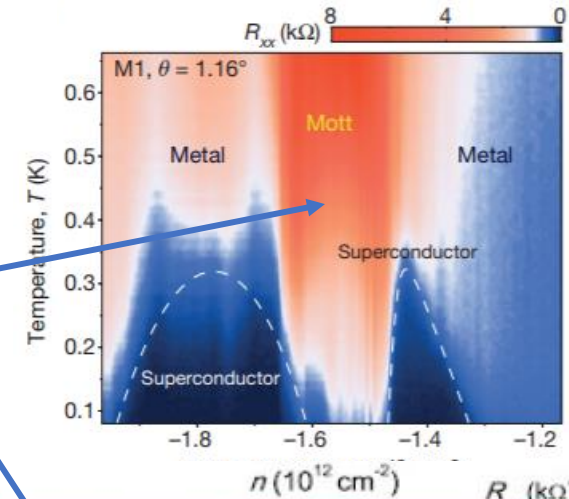
Carr et. al., PRR 1 033072 (2019)

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Theoretical descriptions of twisted bilayer graphene

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Correlated insulators

Cao et. al., Nature 556, 43 (2018)

SC domes

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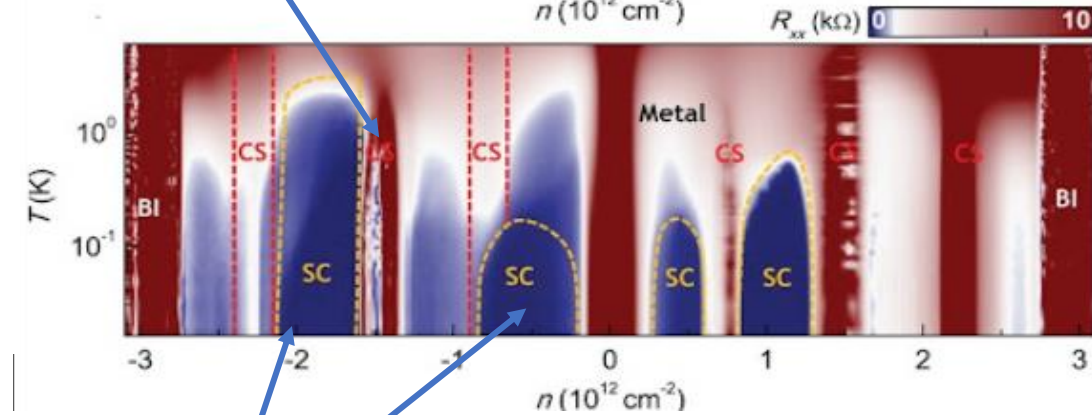
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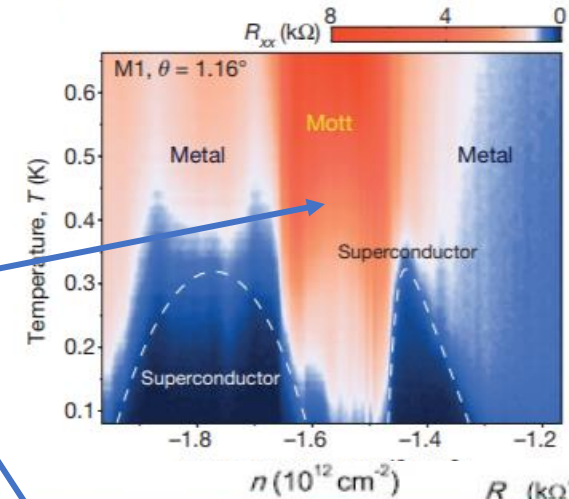
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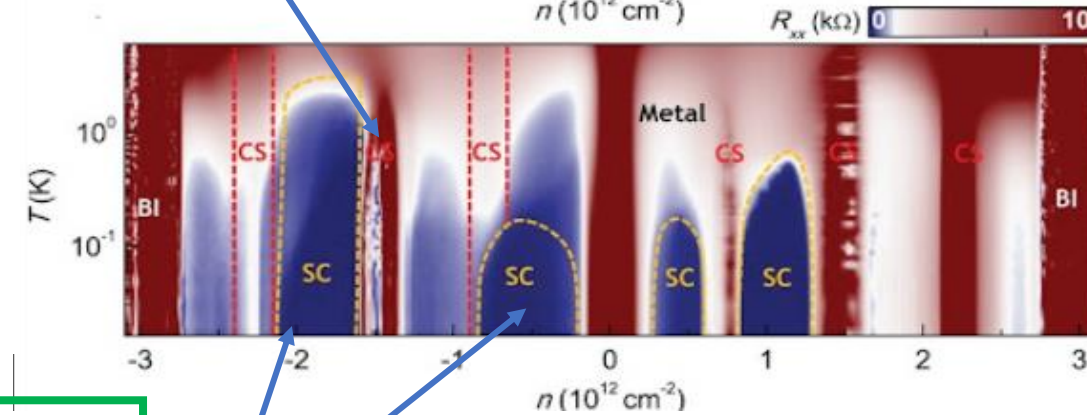
SC domes

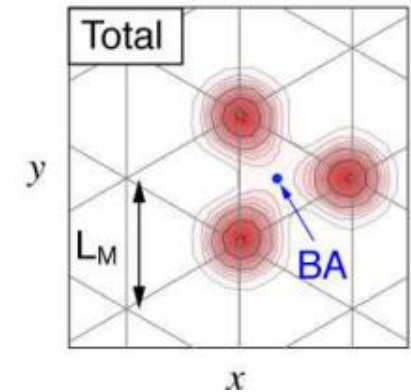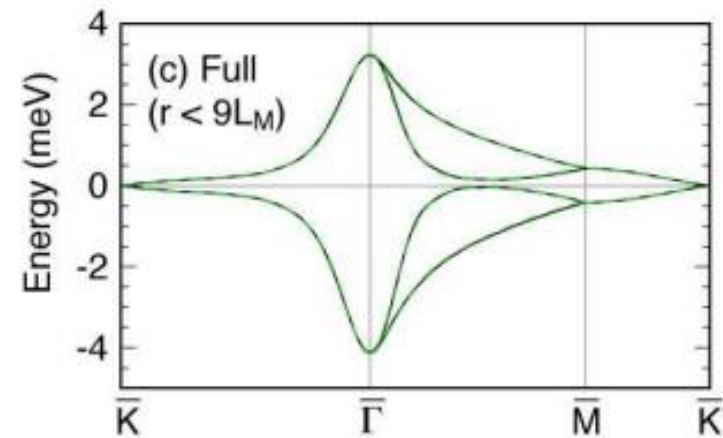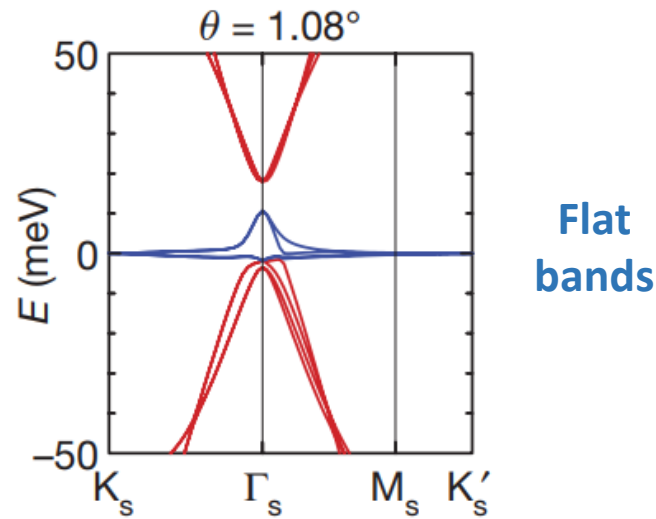Lu et. al., Nature 574, 653 (2019)

➤ **Strong correlation (Mott physics) better captured within interaction models based on effective Wannier function...**

Moiré Wannier orbitals for twisted bilayer graphene

Proposed models with effective moiré Wannier functions

↓

2 Wannier orbitals per valley

Flat bands

Cao et. al., Nature 556, 80 (2018)
Bistritzer and Macdonald, PNAS 108, 12233 (2011)
Suarez Morell et. al., PRB 82, 121407 (2011)

➢ **Very long range interactions**
➢ **Symmetry/topology issues**
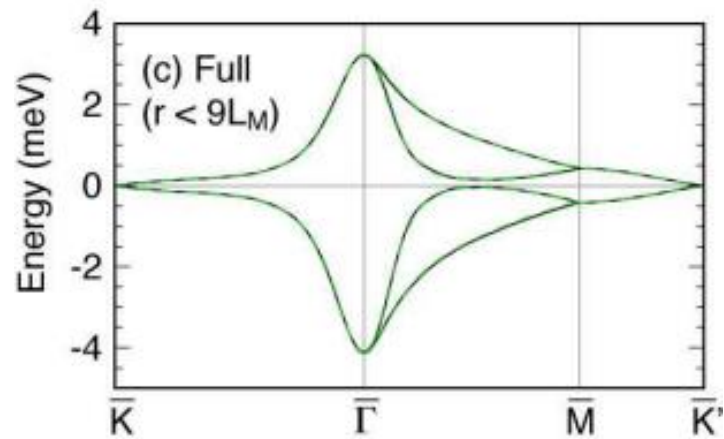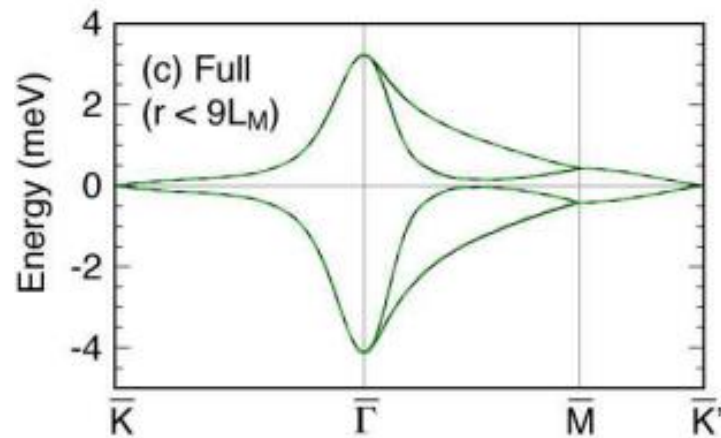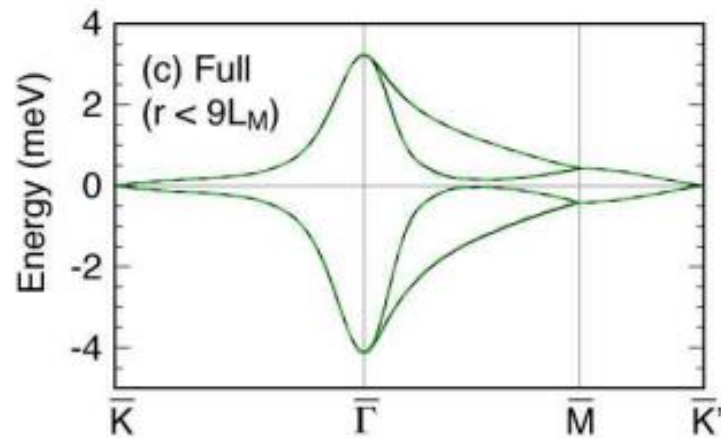
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Proposed models with effective moiré Wannier functions

2 orbitals per valley

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- ➤ **Very long range interactions**
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5, 6, 8, and 10 orbitals per valley
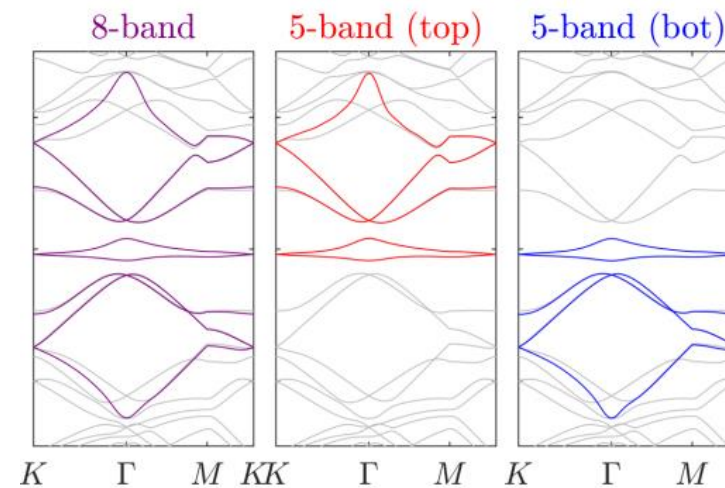
Hoi Chun Po et. al., PRB 99, 195455 (2019)
Carr et. al., PRR 1 033072 (2019)
Carr et. al., PRR 1 013001 (2019)

Moiré Wannier orbitals for twisted bilayer graphene
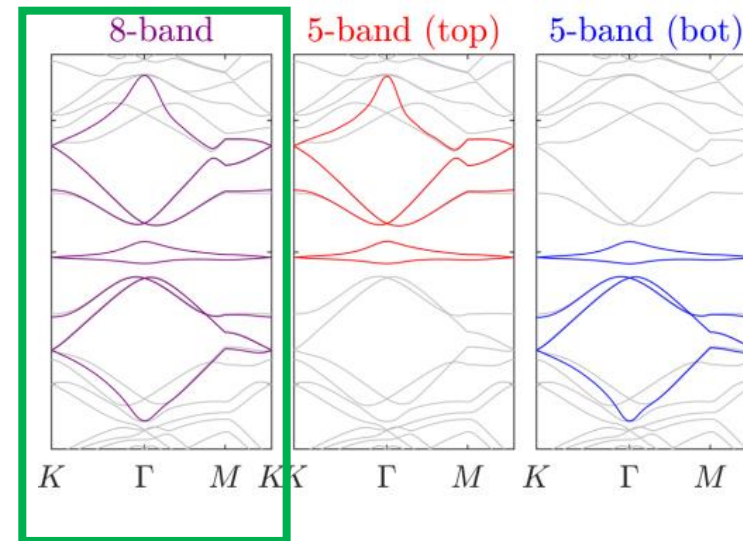
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Hoi Chun Po et. al., PRB 99, 195455 (2019)
Carr et. al., PRR 1 033072 (2019)
Carr et. al., PRR 1 013001 (2019)

BM model with and without PH symmetry breaking term

➢ **Particle-hole symmetry in the Bistritzer-Macdonald model**

$$H = -i\hbar v_f \cos\left(\frac{\theta}{2}\right)\sigma \cdot \eth \mp iv_f\hbar \sin\left(\frac{\theta}{2}\right)(\hat{\sigma} \times \eth)$$

=1

$+ \begin{pmatrix} 0 & T(r) \\ T^+(r) & 0 \end{pmatrix}$ =0

Interlayer coupling; T(r)=T(r)(W0, W1)

Coupling between AA/BB

Coupling between AB

➢ **Topological energy bands with both P and $C_{2z}T$ symmetries, which are gapped from other bands.**

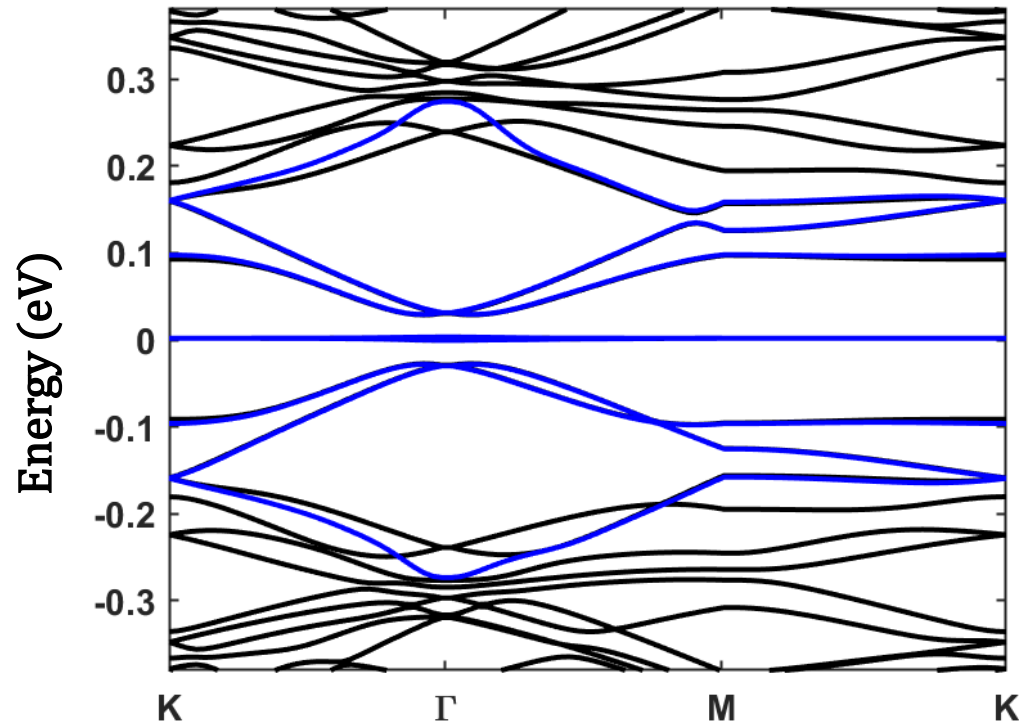Song et. al., PRB 103, 205412 (2021)
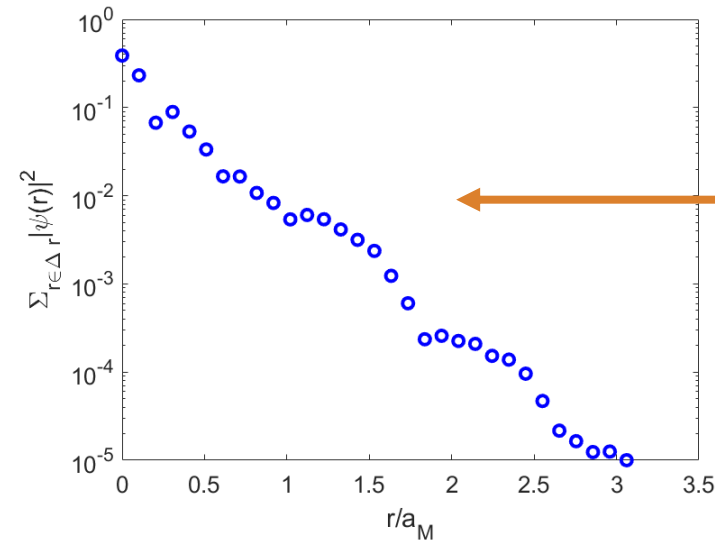

PH symmetric
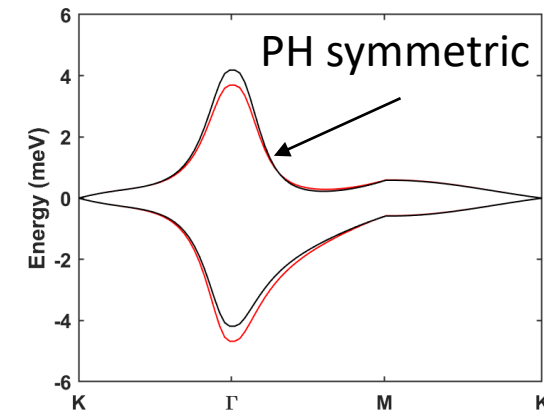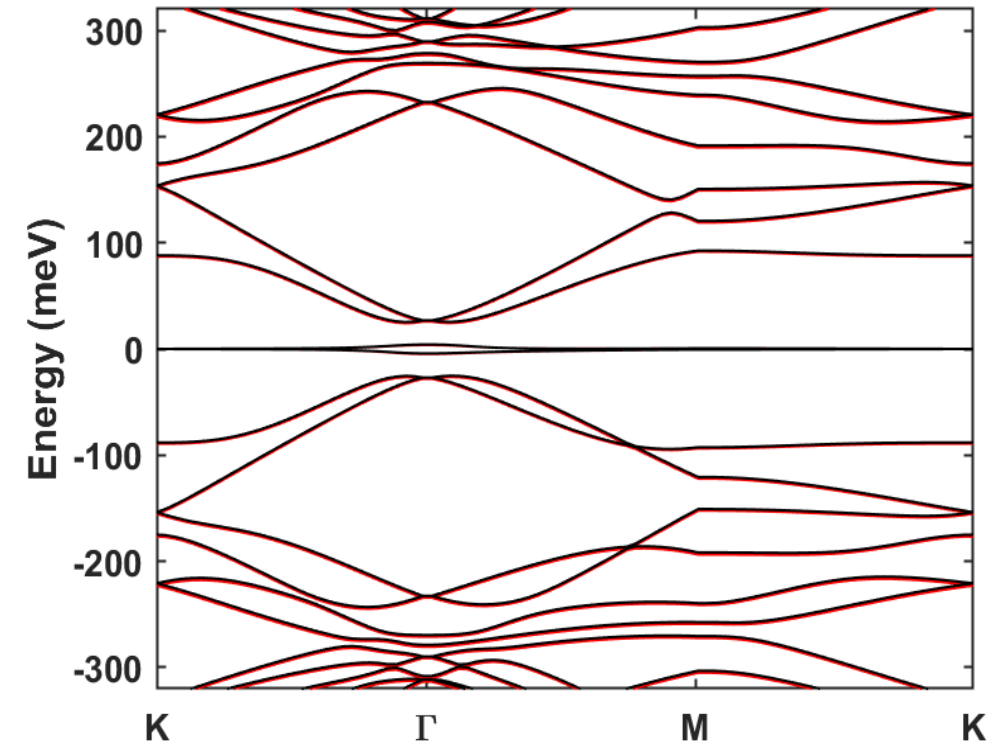
Wannier description for Bistritzer-Macdonald model

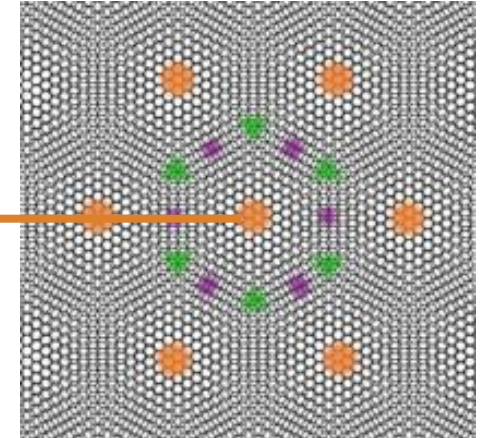**$W_0/W_1=0.78$; $W_1=110$ meV**

Probability density of Wannier functions Vs distance

Exponential localization of Wannier functions

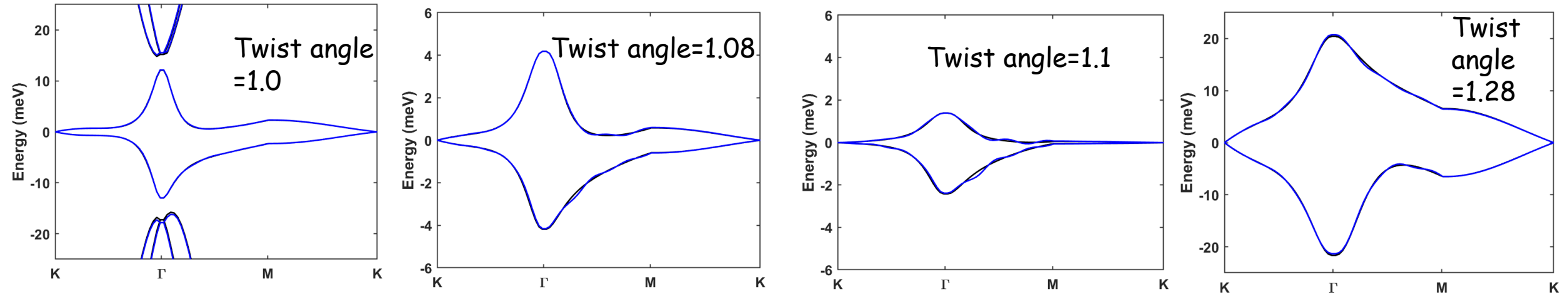**Wannier orbitals in moiré superlattice**

At AA: 3 orbitals with 'p+', 'p-', 's' symmetries

At AB/BA: 2 orbitals with 'pz' symmetry
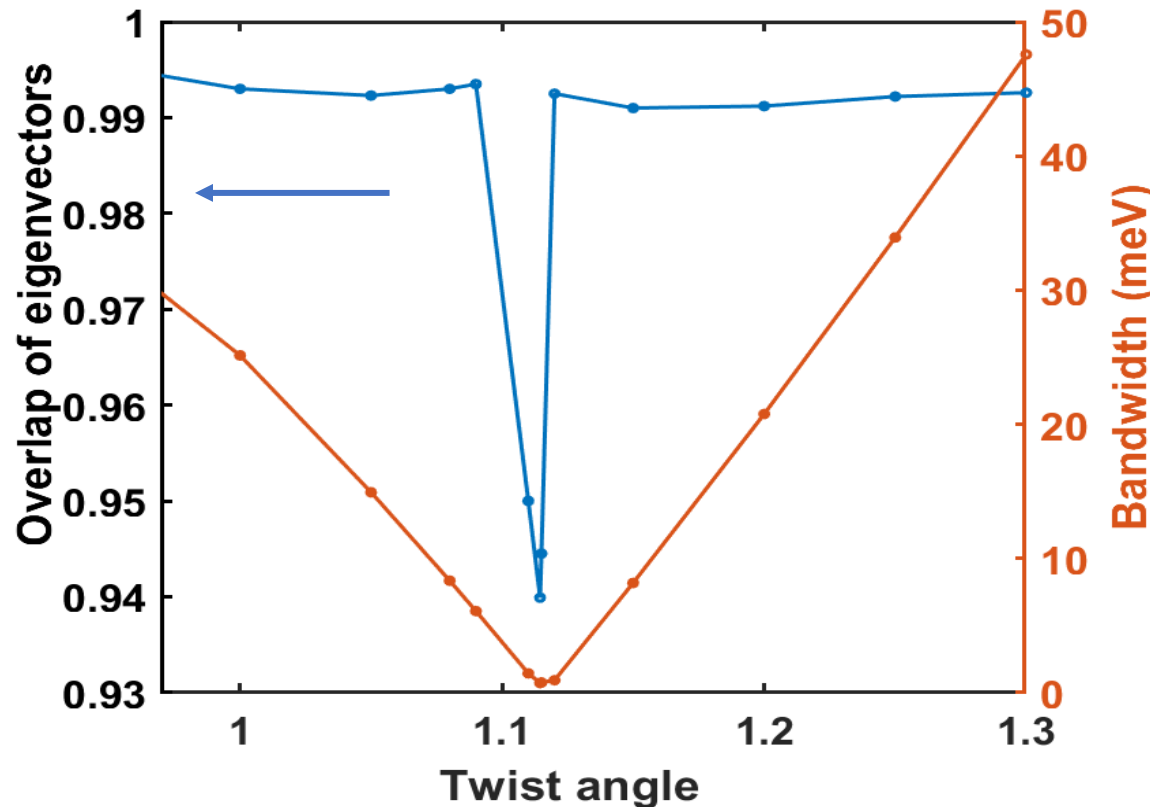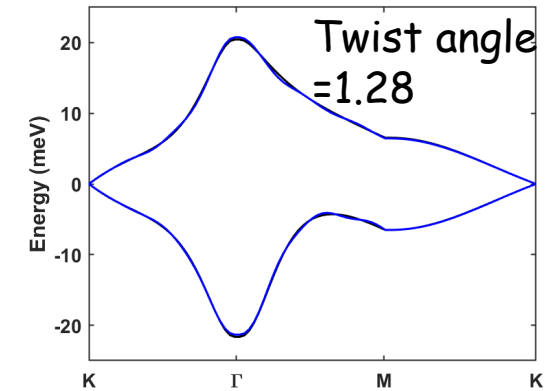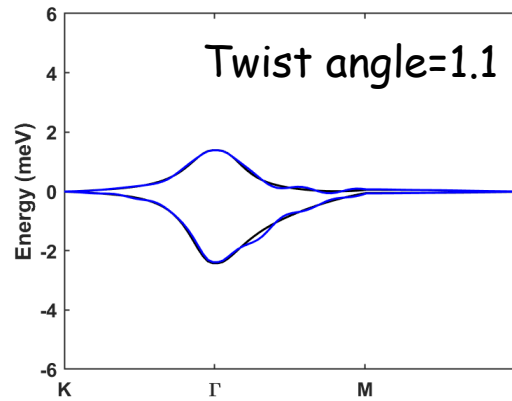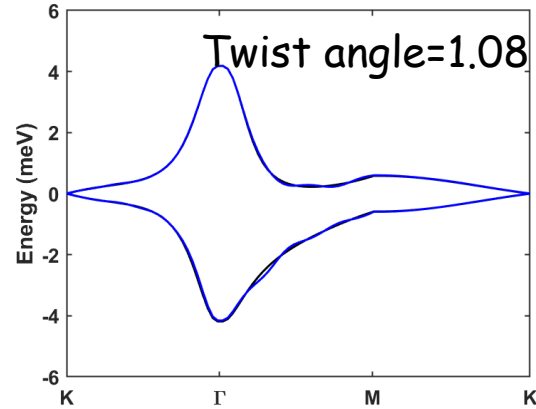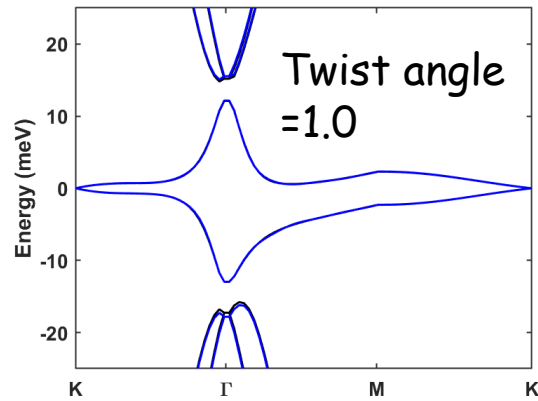
intermediate stacking: 3 orbitals with 's' symmetry

➤ **Without the particle-hole symmetry breaking term (θ dependent term in Dirac Hamiltonians)**

➤ **Symmetries: (C_2T (180^0 rotation + time reversal), C_3(120^0 rotation), M_x (mirror symmetry); particle-hole symmetry is not imposed for the Wannieization.**

> **Hopping range$=8 L_M$**

Twist angle =1.0

Twist angle=1.08

Twist angle=1.1

Twist angle =1.28

> **Overlap of eigenvectors of the flat bands before and and after Wannierization.**

> **Reasonable value of the overlap expect at a narrow range of twist angles with very small bandwidth.**
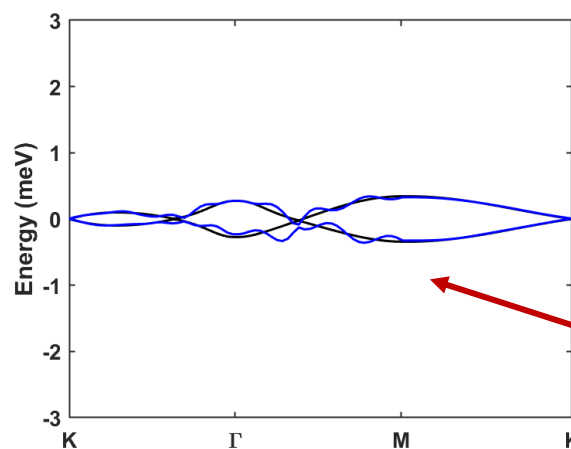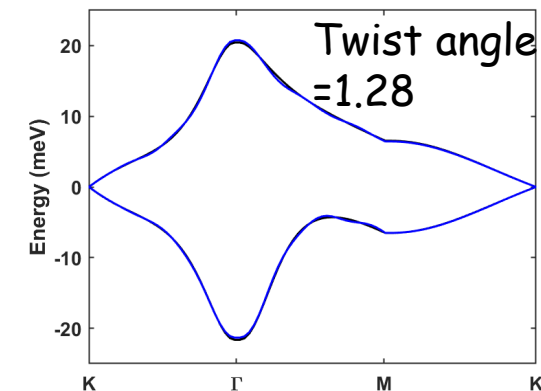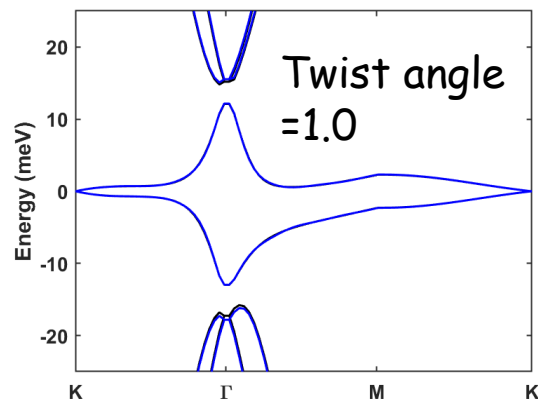
> **Hopping range=$8L_M$**

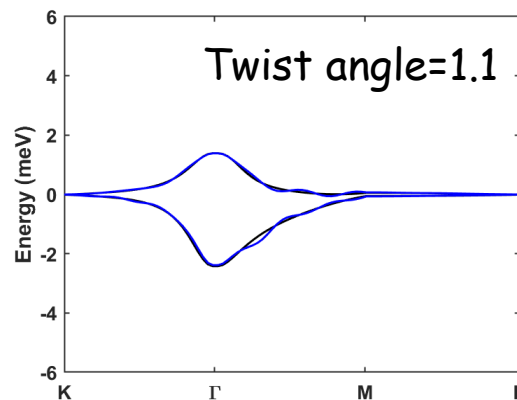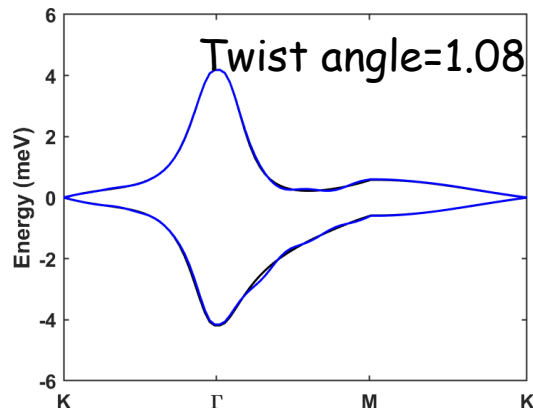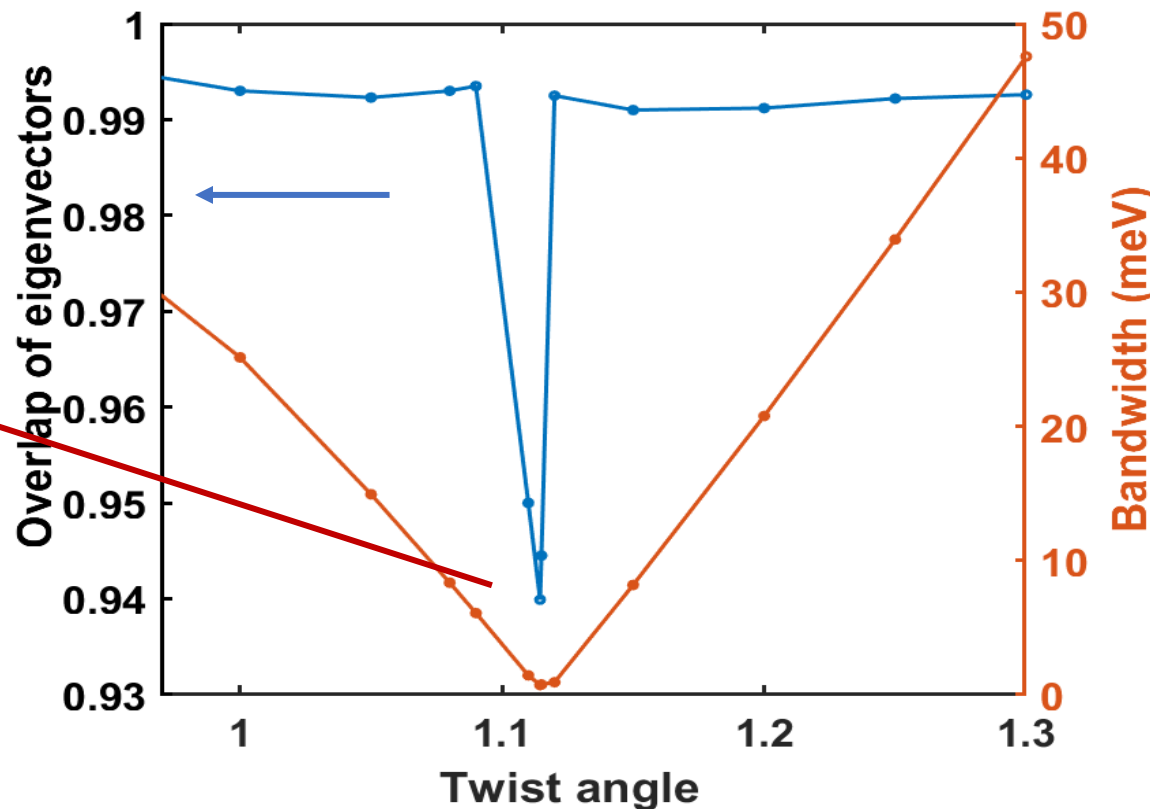$$\text{Overlap}=\sum_k |\langle u_{(k)}^{BM}|u_{(k)}^{\omega an}\rangle|^2$$

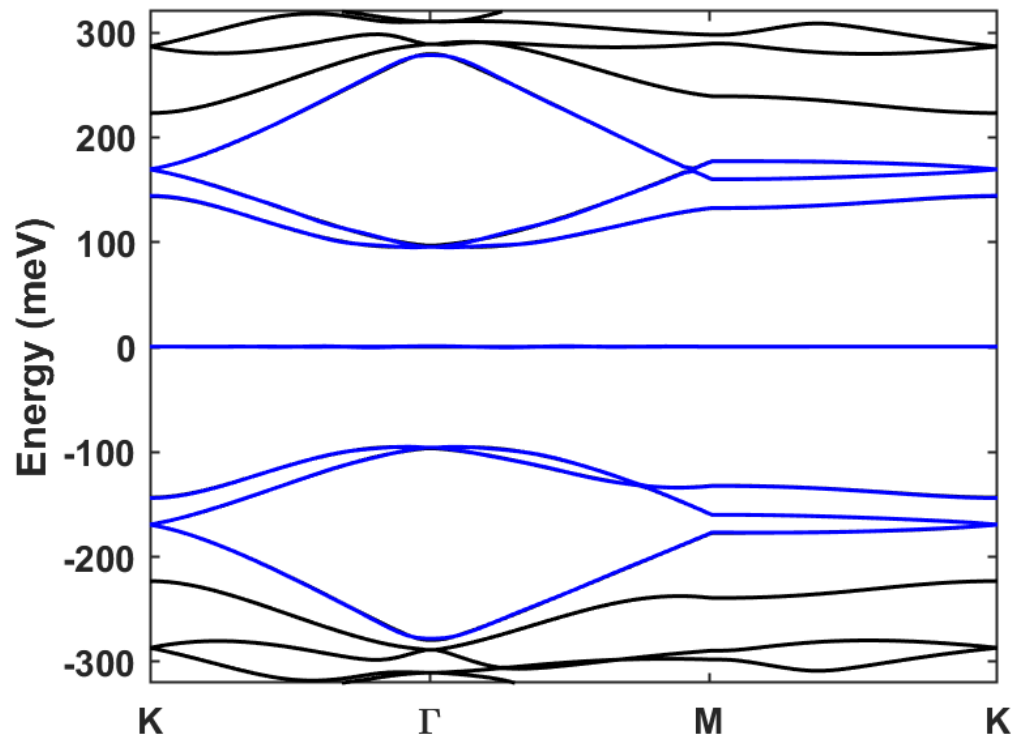$$U_{(k)}^{\omega an} = \sum_\alpha C_n^\alpha(k) |k,\alpha>$$

orbital   band

Comparison of the bands after Wannierization with the bands from the Bistritzer-Macdonald model $W_0/W_1=0.78$

Twist angle =1.0

Twist angle=1.08

Twist angle=1.1

Twist angle =1.28

Hopping range=$8L_M$

$$\text{Overlap}=\sum_k |\langle u_{(k)}^{BM}|u_{(k)}^{\omega an}\rangle|^2$$

$$U_{(k)}^{\omega an} = \sum_\alpha C_n^\alpha(k)\,|k,\alpha>$$

orbital   band

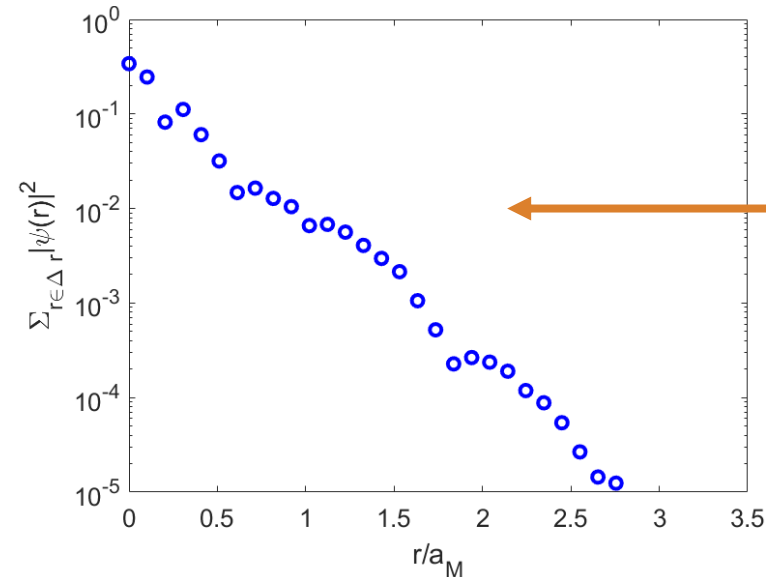range of twist angles with very small bandwidth.

$W_0/W_1=0.2$

Probability density of Wannier functions Vs distance

Wannier orbitals in moiré superlattice

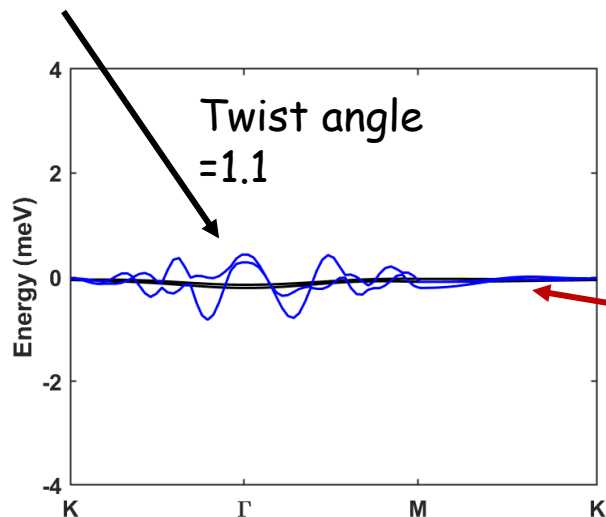**Exponential localization of Wannier functions**

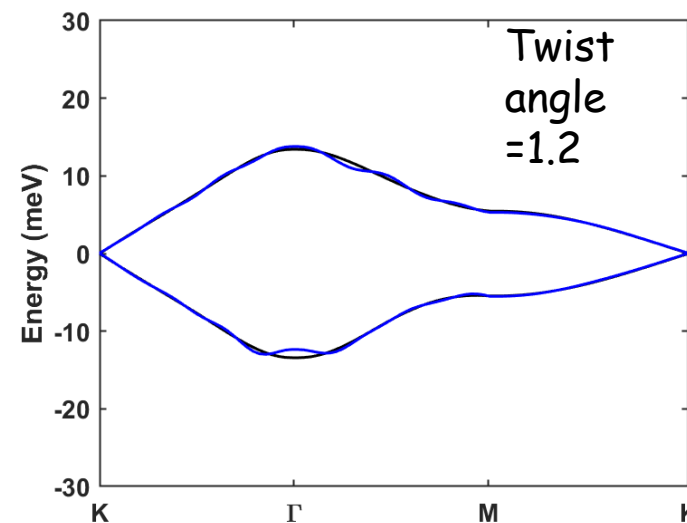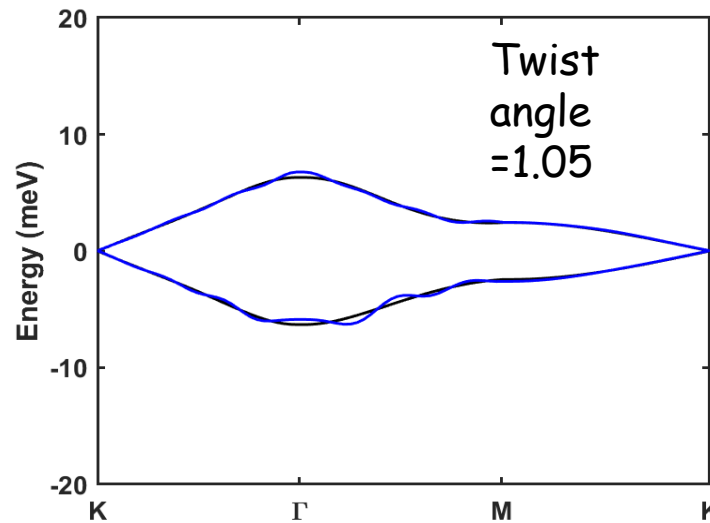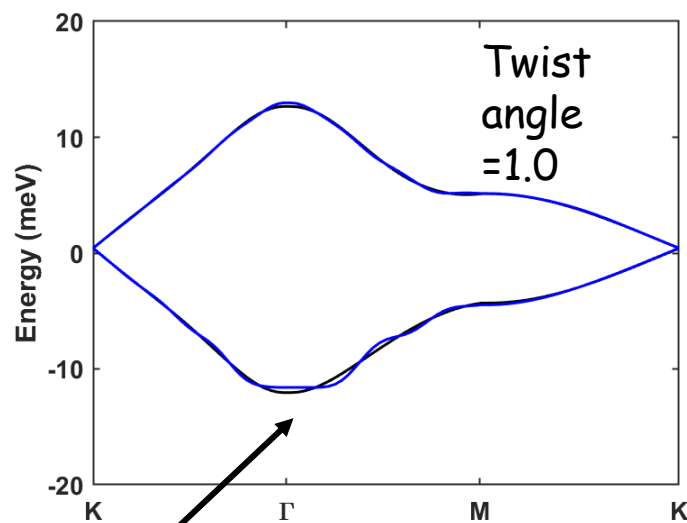At AA: 3 orbitals with 'p+', 'p-', 's' symmetries

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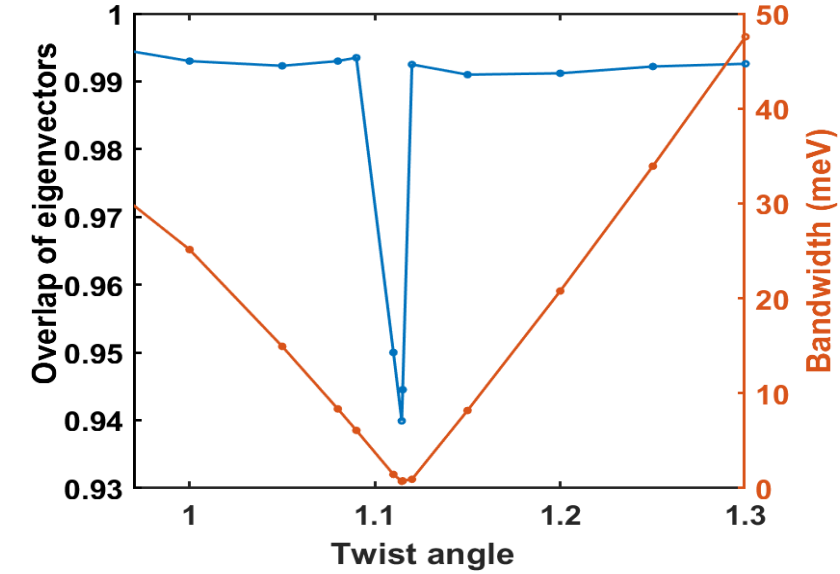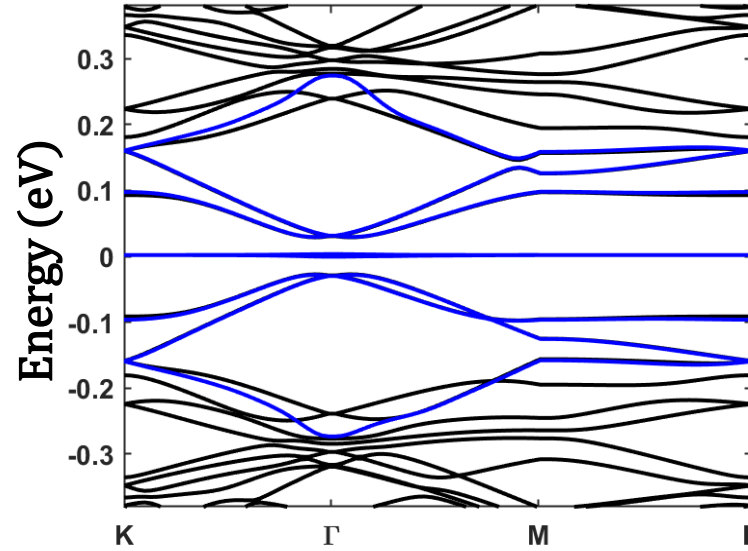
Twist angle =1.0

Twist angle =1.05

Twist angle =1.2

Not optimized

Twist angle =1.1
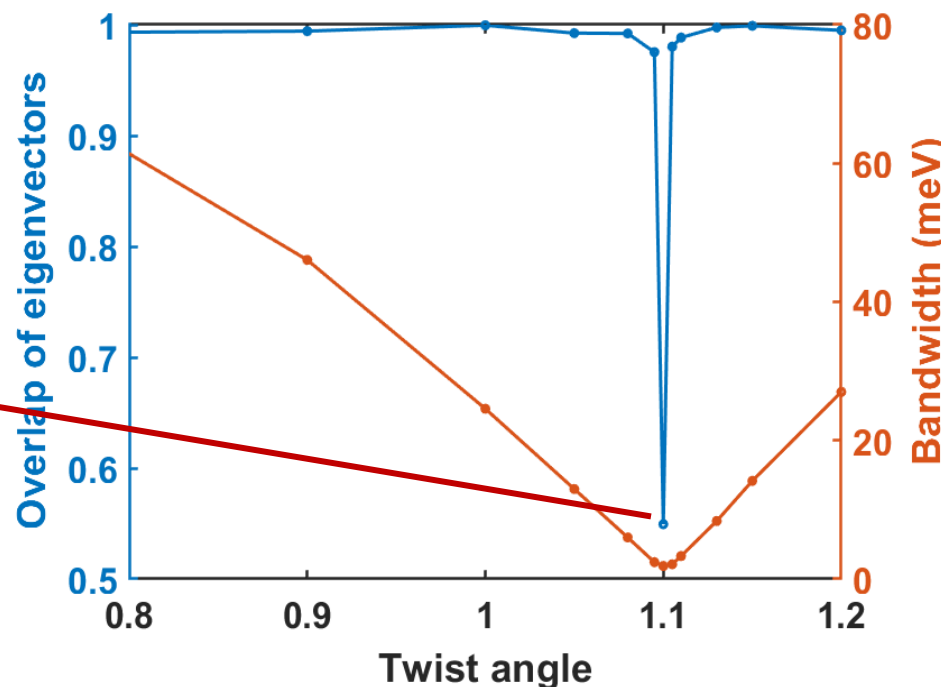
Hopping range=$8a_M$

$$\text{Overlap} = \sum_k |\langle u^{BM}_{(k)} | u^{\omega an}_{(k)} \rangle|^2$$

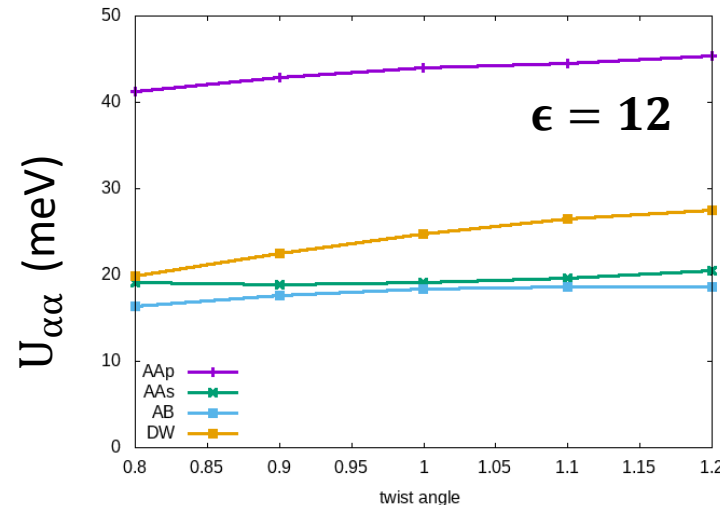$$U^{\omega an}_{(k)} = \sum_\alpha C^\alpha_n(k) |k, \alpha >$$

orbital   band

> **Effective Wannier representation with 8 moiré Wannier orbitals per valley for the Bistritzer-Macdonald model.**

> **Starting point of studying interaction effects in twisted bilayer graphene..**

Onsite intra-orbital density-density interactions

BM model, W0/W1=0.78

Thank you!