An accurate tight binding model for twisted bilayer graphene describes topological flat bands without geometric relaxation

https://arxiv.org/abs/2110.03508

Shivesh Pathak[1], Tawfiqur Rakib[2], Run Hou[3], Andriy Nevidomskyy[3], Elif Ertekin[2], Harley T. Johnson[2], and Lucas K. Wagner[4]
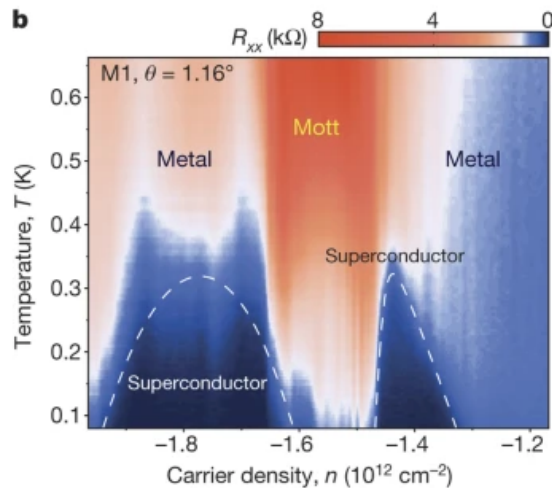
1. Sandia National Labs, sapatha@sandia.gov
2. Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign
3. Department of Physics and Astronomy, Rice University
4. Department of Physics, University of Illinois at Urbana-Champaign

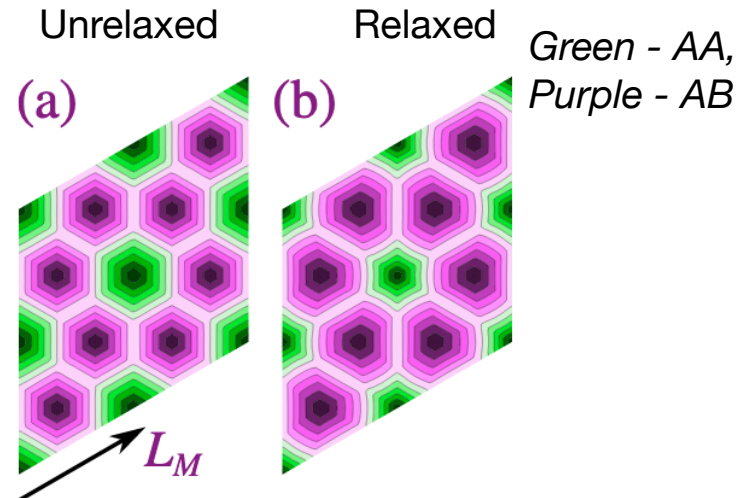# Structural-electronic interaction in TBLG

Novel behavior at magic twist angle: 1.05 degrees

Electronic structure

Cao *et al.* Nature (2018)

Lattice relaxation

Unrelaxed   Relaxed   *Green - AA, Purple - AB*

Guinea and Walet, PRB (2019)

STM measurements: Jiang *et al.* Nature (2019)

How does the lattice structure affect the low-energy electronic structure?

Low-energy electronic structure: bands and interactions

We can break the electronic structure problem into two pieces

Band structure

How does the lattice structure affect the bands near Fermi level?

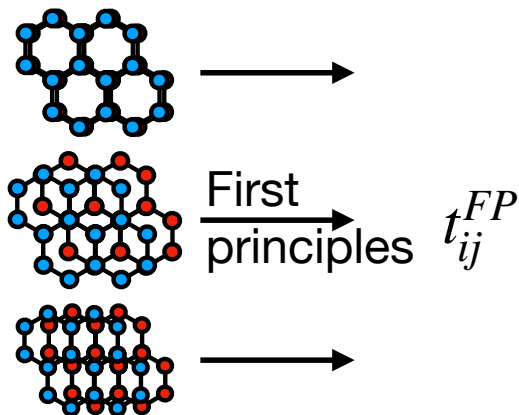**Electron-electron interactions**

How does the lattice structure affect the low-energy effective interactions?
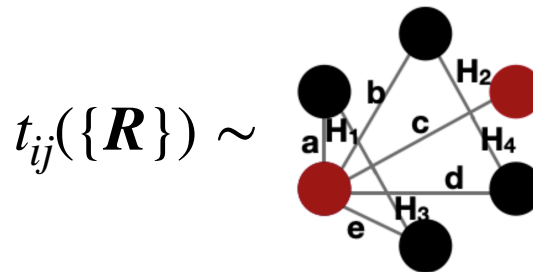
The project, at a glance

What does a more accurate TB model for TBLG look like?
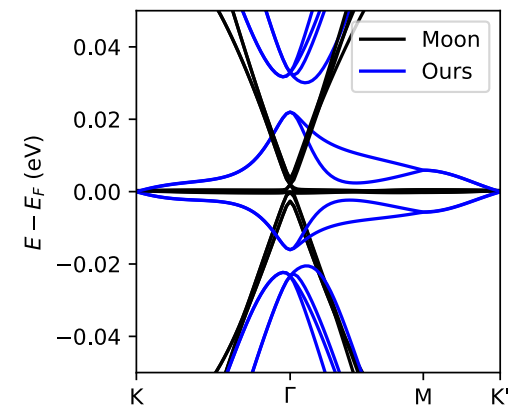What does the model tell us about how the lattice affects band structure?

Generate first principles training data

Fit a local environment tight binding model (LETB)

Use LETB to study structure-band interaction

$$t_{ij}^{FP}$$

First principles

$$t_{ij}(\{\boldsymbol{R}\}) \sim$$

Parameterization - local environment tight binding (LETB)

$$t_{ij}(\{\boldsymbol{R}\}, \boldsymbol{p})$$
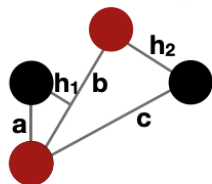
Intralayer hoppings

Nearest neighbor
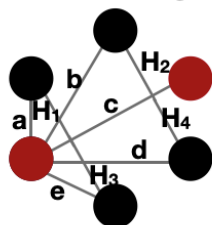

$t_{01} \sim a$

2 parameters

Second nearest neighbor

$t_{02} \sim a, b, c, h_1, h_2$
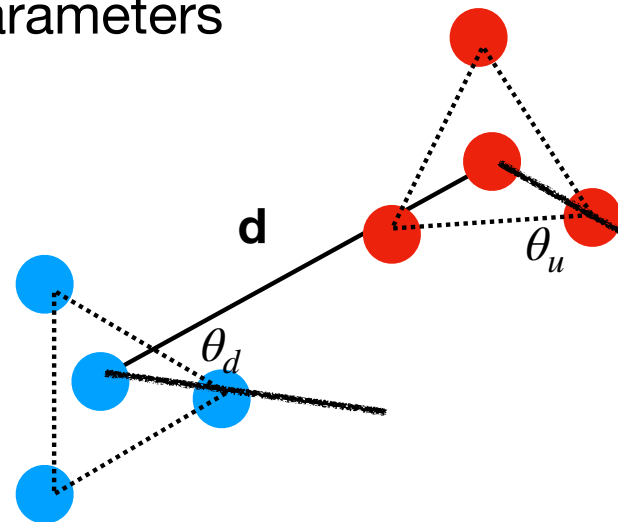
6 parameters

Third nearest neighbor

$t_{03} \sim a, b, c, d, e, H_1, H_2, H_3, H_4$
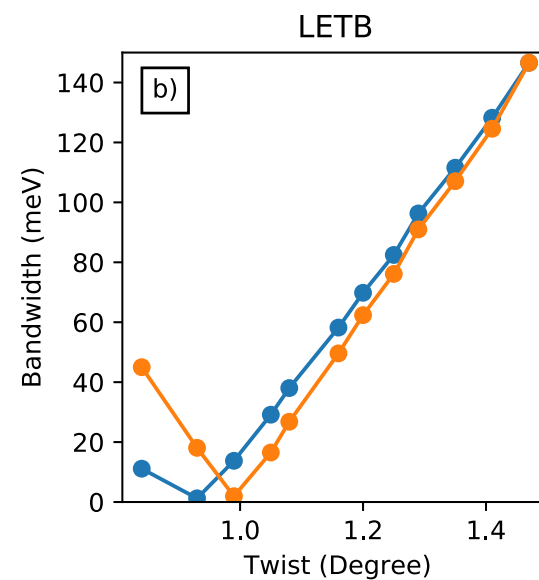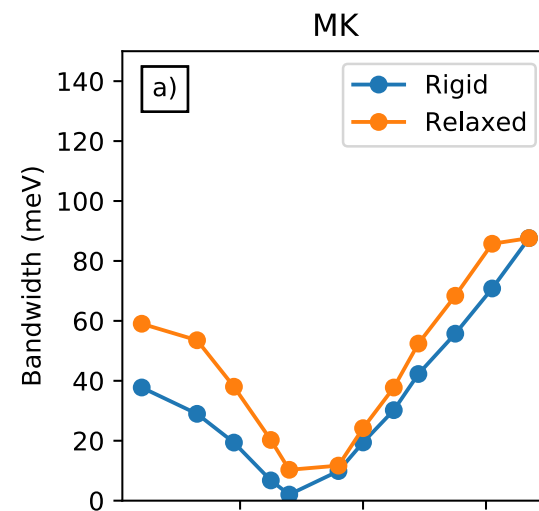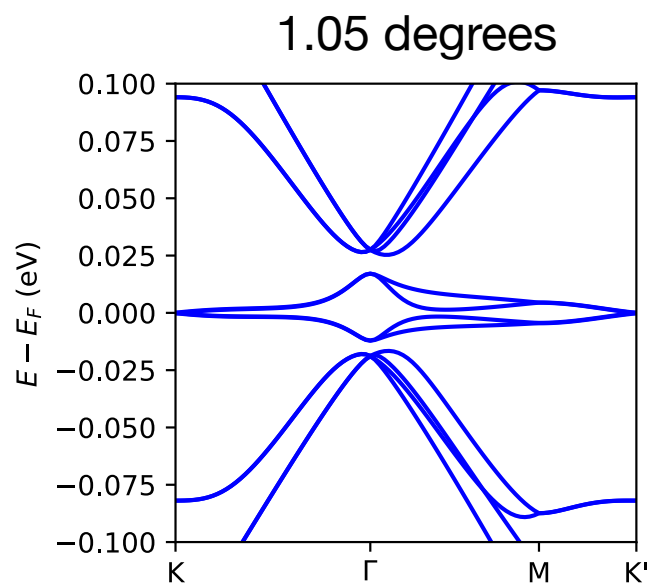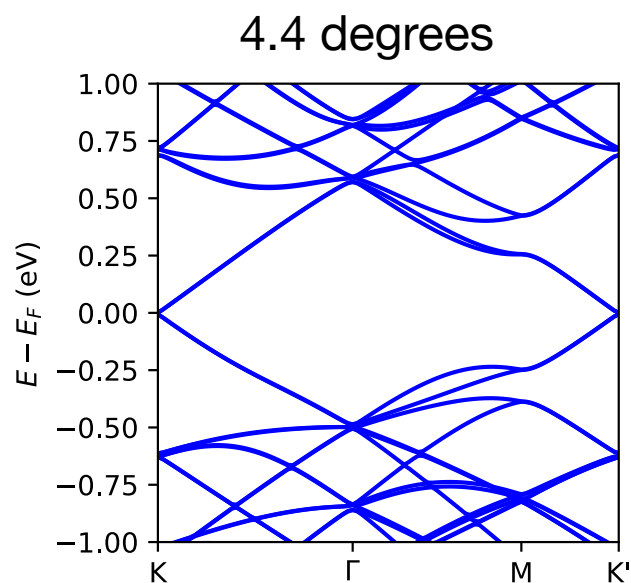
10 parameters

Interlayer hoppings

$t_{inter} = f^{Fang}(d, \theta_u, \theta_d)$ Fang and Kaxiras *et al.* ArXiV (2019)

10 parameters

Band flattening in LETB

Rigidly twisted bilayer graphene

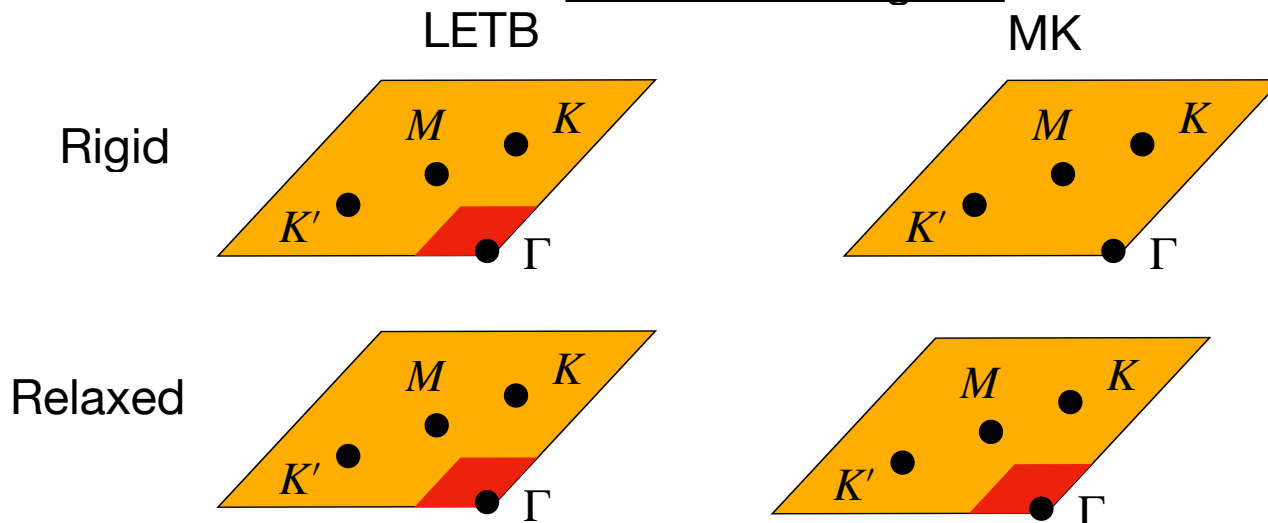# Topological flat bands

Topology ~ Localization (Wannier) obstruction
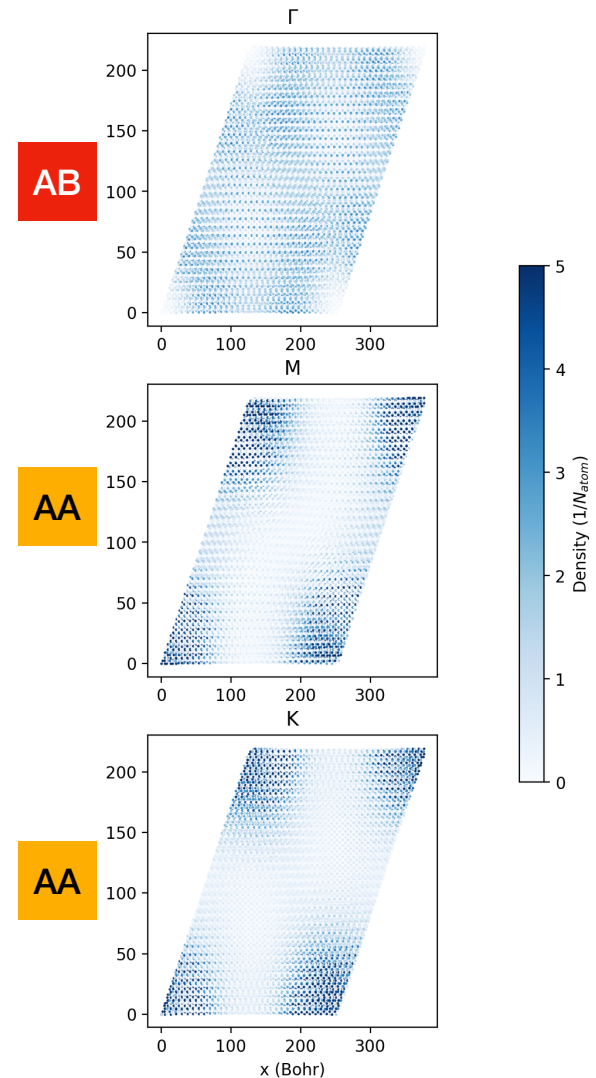
Study the orbitals across the 1BZ at 1.05 degrees

1BZ at 1.05 degrees

LETB   MK

Rigid

Relaxed

MK model - topological flat bands require relaxation
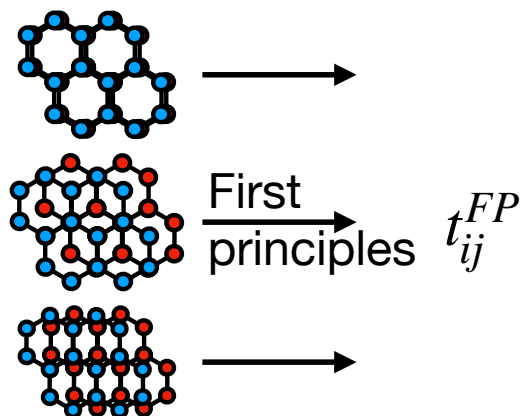LETB - topological flat bands even with rigid twist!

Rigid twist, LETB

Project summary
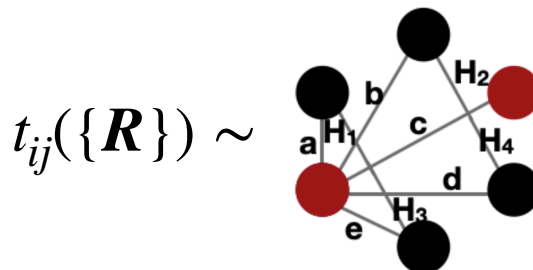
What does a more accurate TB model for TBLG look like?
What does the model tell us about how the lattice affects band structure?

**Bonus:
Publishable data
and model!**

**Generate
first principles
training data**

**Fit a local
environment tight
binding model
(LETB)**

**Use LETB to study
structure-band
interaction**