QMC-HAMM: A highly accurate local environment tight-binding model LETB for twisted bilayer graphene

qmc-hamm.github.io

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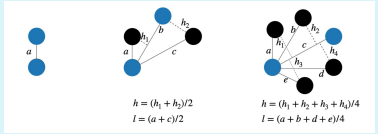
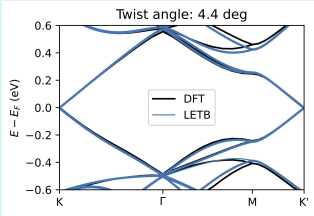
Position-dependent tight binding

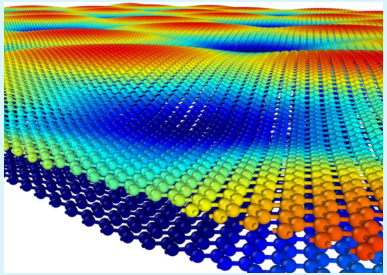


Minimal descriptors selected using LASSO feature selection algorithm.



Accurate reproduction of DFT band structure.

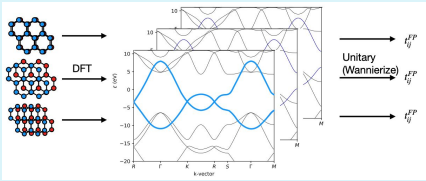
The need:



Twisted bilayer graphene buckles and distorts, which affects the electronic structure.

How do the distortions affect the flat bands and topological character of the system?

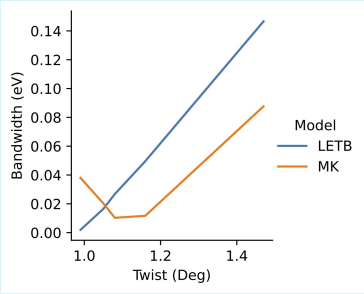
The approach



73 random configurations, including shear and displacements of the atoms. Common commensurate structure, such as AB, SP, AA stacked graphene are included.

Each configuration has 128 tight-binding parameters between all pairs of atoms, resulting in 9344 tight-binding parameters to fit.

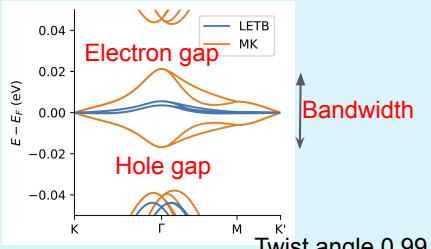
Effects of a more accurate model



Minimum in bandwidth at 'magic angle' may be accidental in simpler TB models.

Moon, Koshino. Phys. Rev. B 85, 195458 (2012)

Difference in band structure



Twist angle 0.99

Software package

```
import ase
from bilayer_letb.api import tb_model

ase_atoms = ase.io.read_cif("twisted_graphene.cif")
letb = tb_model(ase_atoms)
# Compute bands
k=[[1/3., 2/3.], [0.0, 0.0], [0.5, 0.0], [2/3., 1/3.]]
(k_vec, k_dist, k_node) = letb.k_path(k, 100)
evals = letb.solve_all(k_vec)
```

pip install bilayer_letb