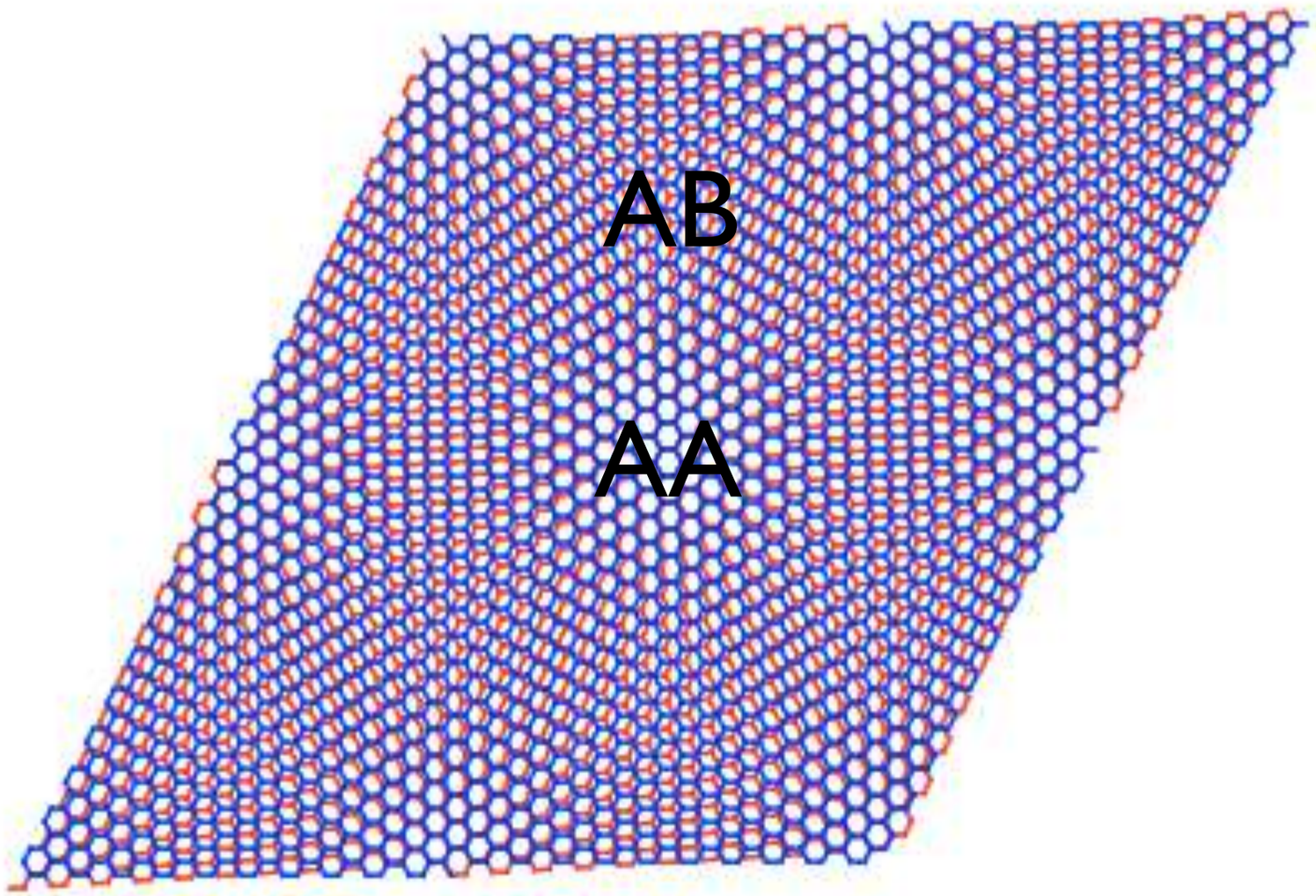
ELECTRONIC PROPERTIES OF TWISTED BILAYER GRAPHENE

Johannes Lischner

Imperial College London

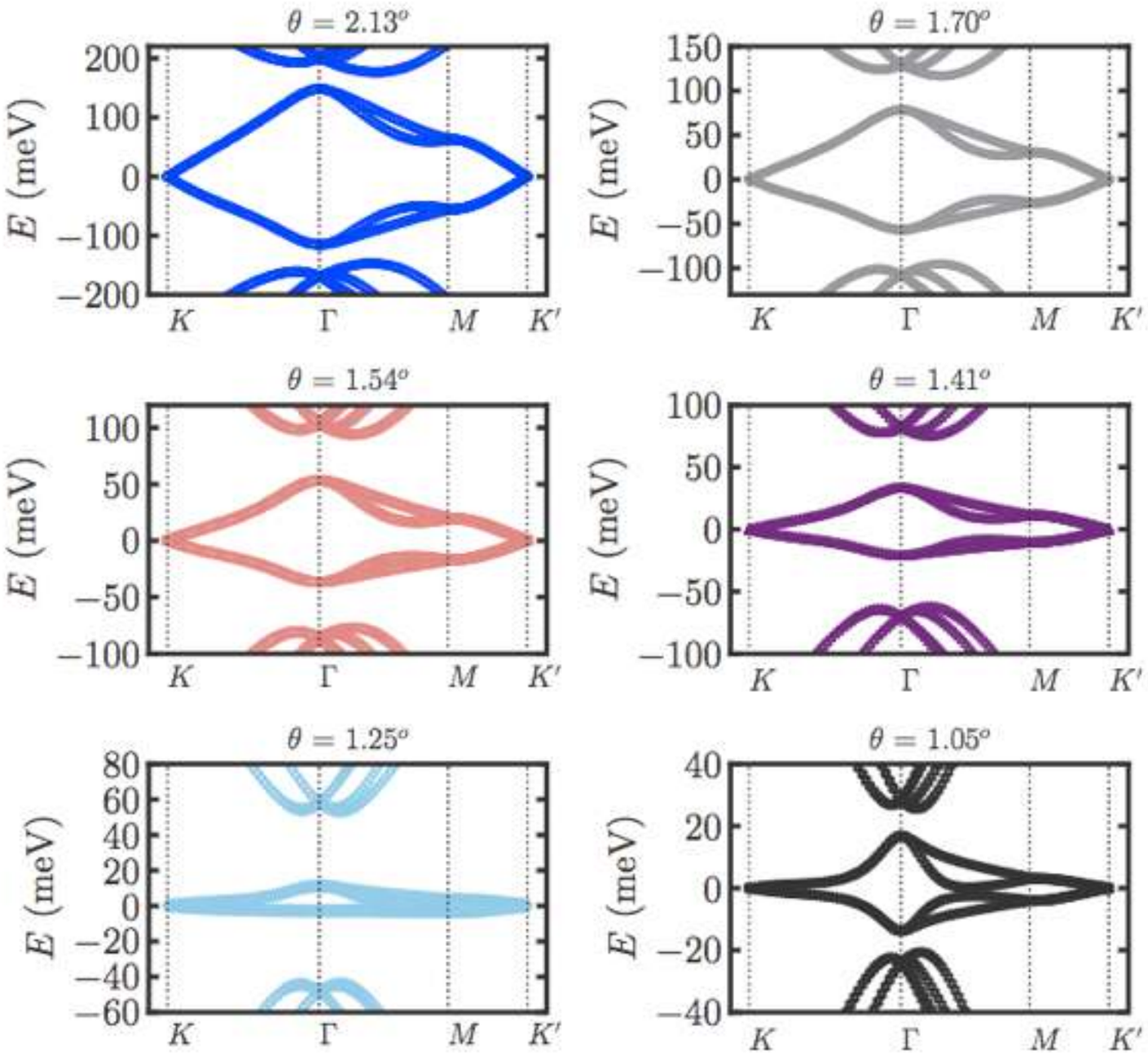
TWISTED BILAYER GRAPHENE

a moire material



TWISTED BILAYER GRAPHENE

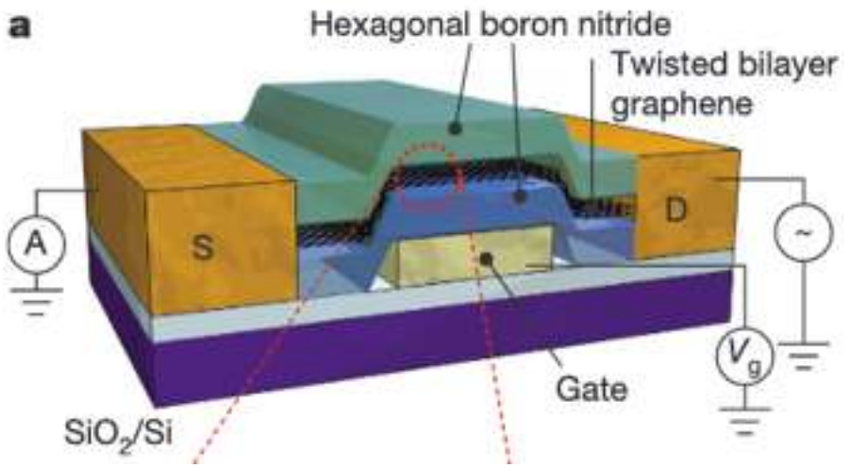
theory predicts (2011): flat bands at magic angle

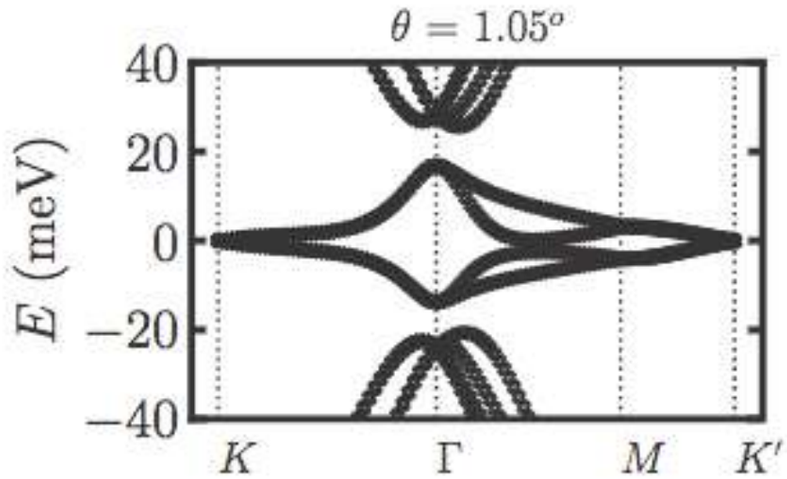


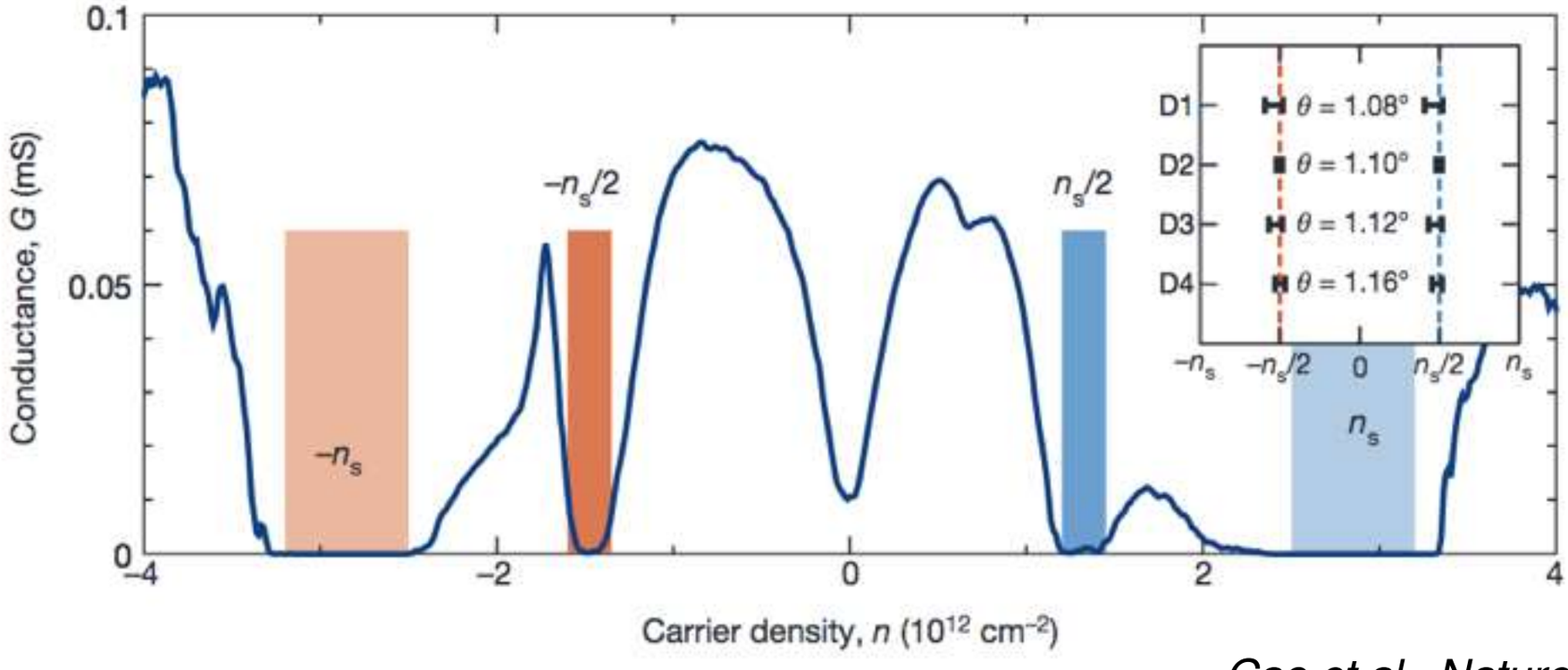
Bistrizer, MacDonald, PNAS 108, 412233(2011)

TWISTED BILAYER GRAPHENE

experiment catches up (2018)



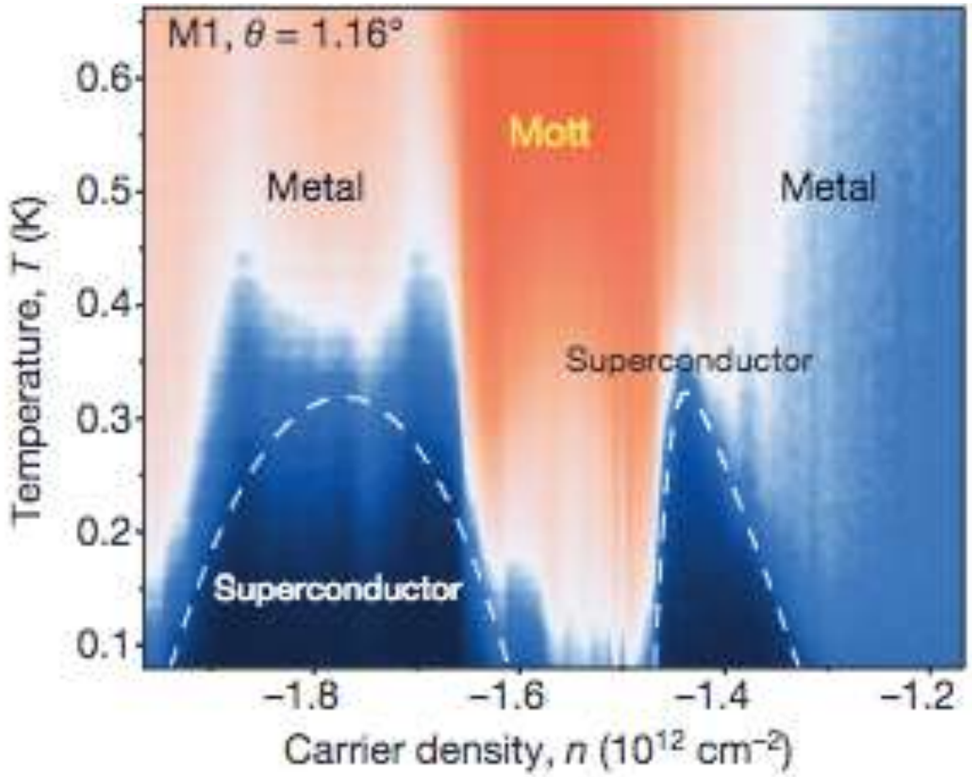


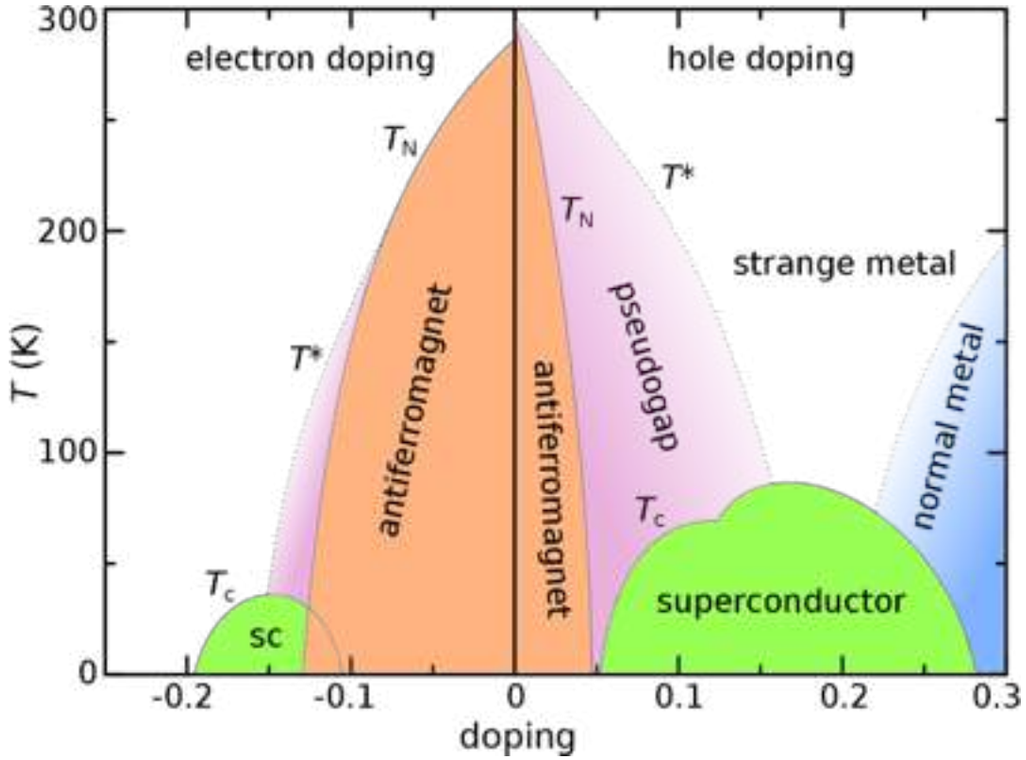


Cao et al., Nature 556, 80 (2018)

TWISTED BILAYER GRAPHENE

phase diagram similar to cuprates

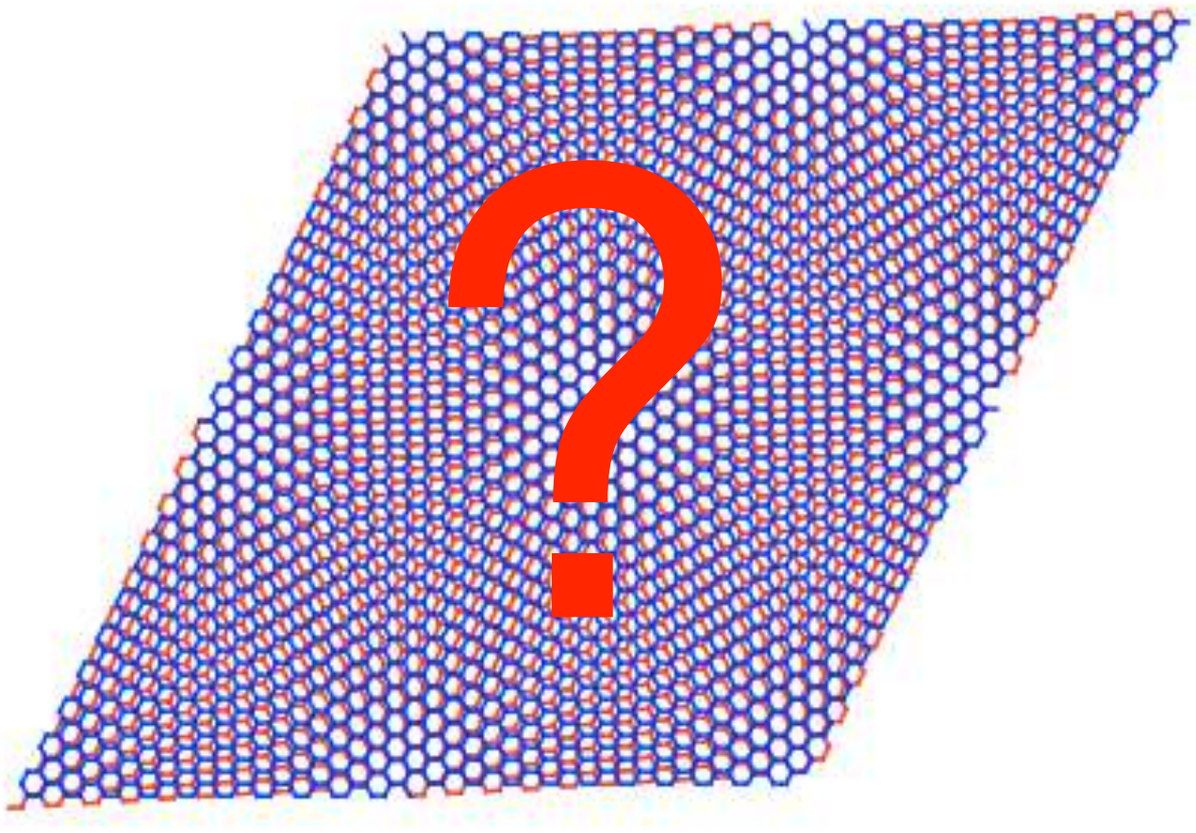




Cao et al., Nature 556, 43 (2018)

UNDERSTANDING MOIRE MATERIALS

What is the role of electron-electron interactions?



UNDERSTANDING THE NORMAL STATE

atomistic tight-binding based Hartree theory

$$H = \sum_{ij} t(\mathbf{r}_i - \mathbf{r}_j) c_i^\dagger c_j + \sum_i V_H(\mathbf{r}_i) c_i^\dagger c_i$$

$$V_H(\mathbf{r}) = \int d\mathbf{r}' W(\mathbf{r} - \mathbf{r}')[n(\mathbf{r}') - n_0(\mathbf{r}')]$$

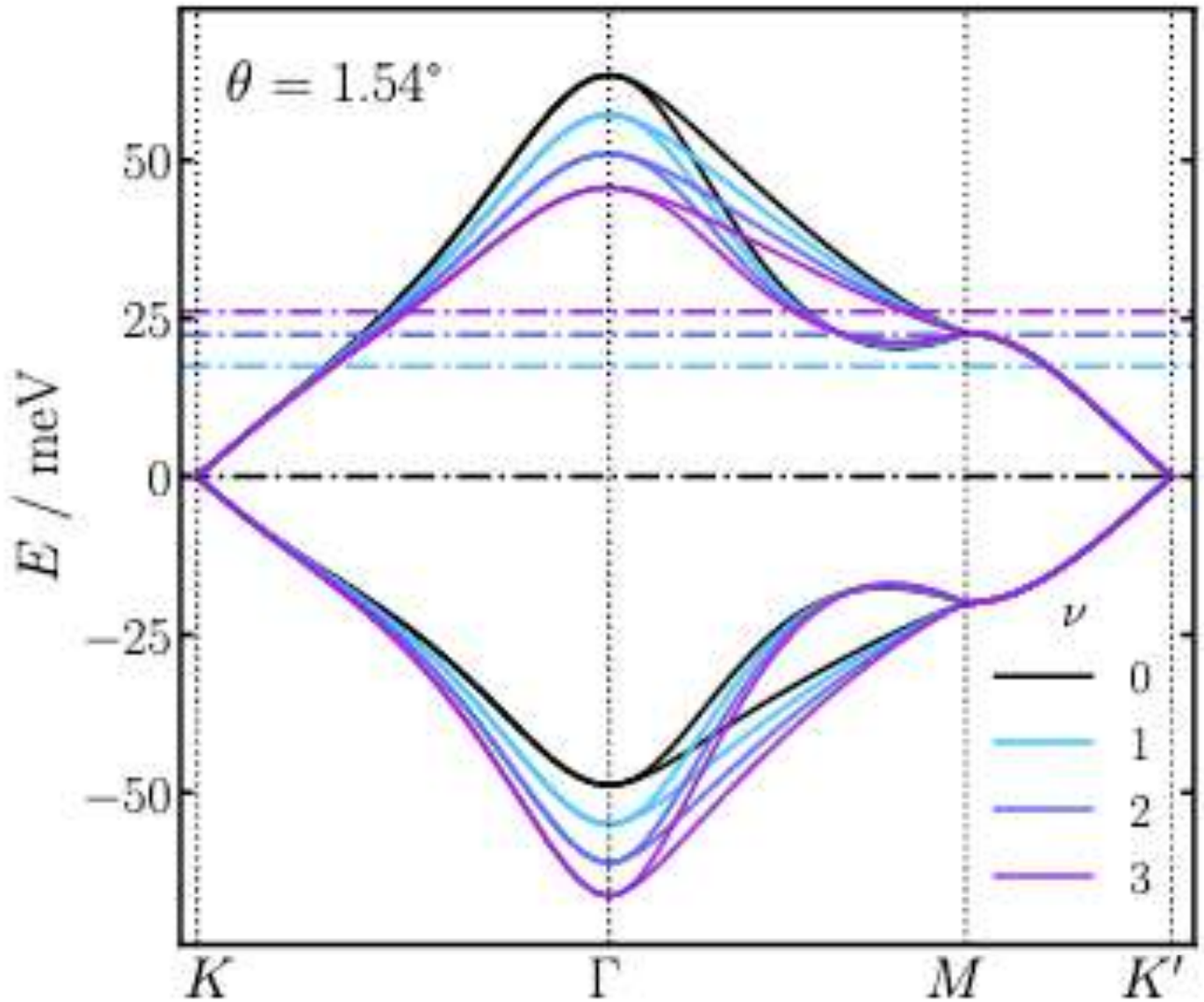
$$W(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0\epsilon_{bg}|\mathbf{r}|}$$

Rademaker et al., Phys. Rev. B 100, 205114 (2019)

Goodwin et al., arXiv:2004.14784

UNDERSTANDING THE NORMAL STATE

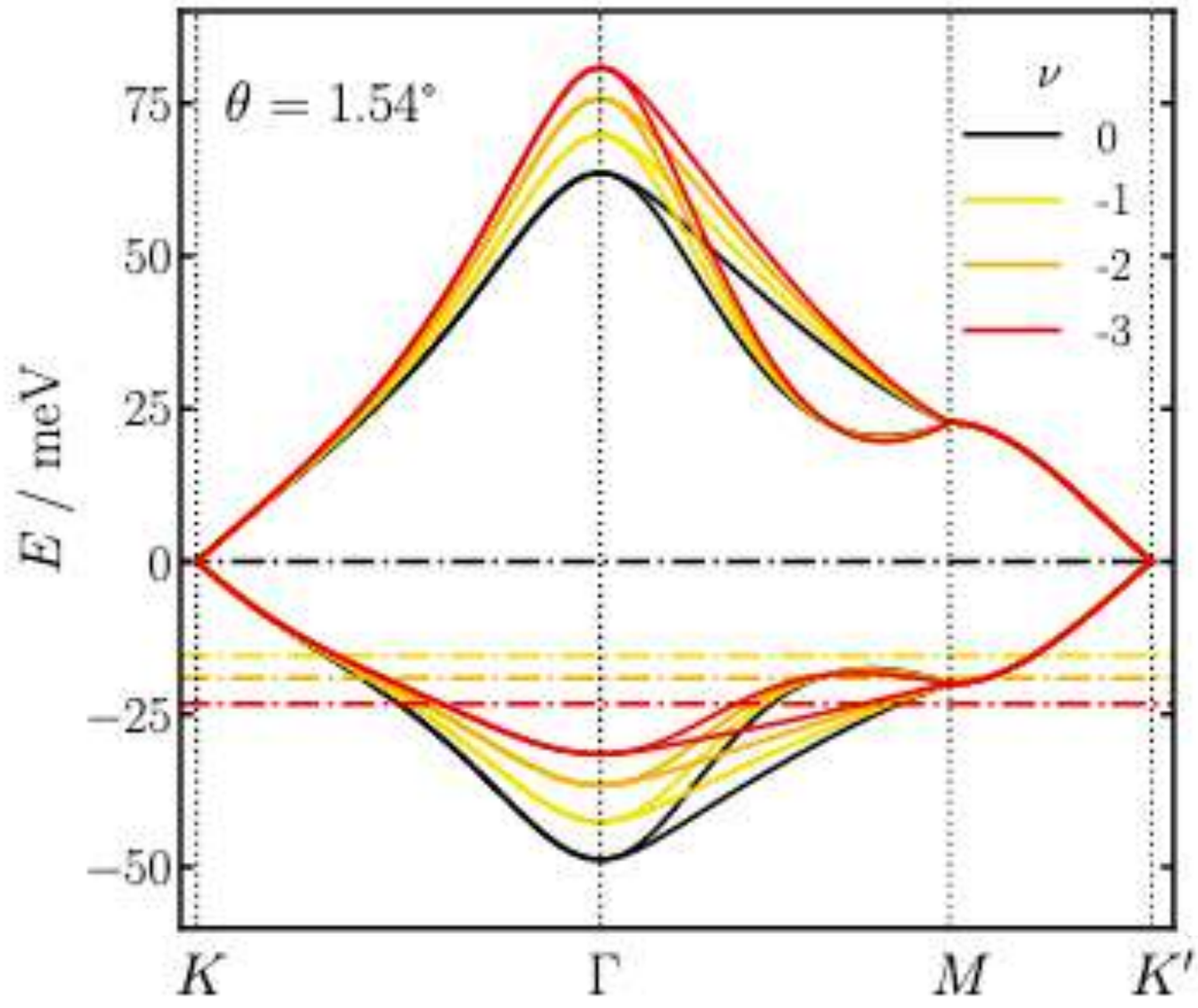
band structure of electron doped tBLG



Goodwin et al., arXiv:2004.14784

UNDERSTANDING THE NORMAL STATE

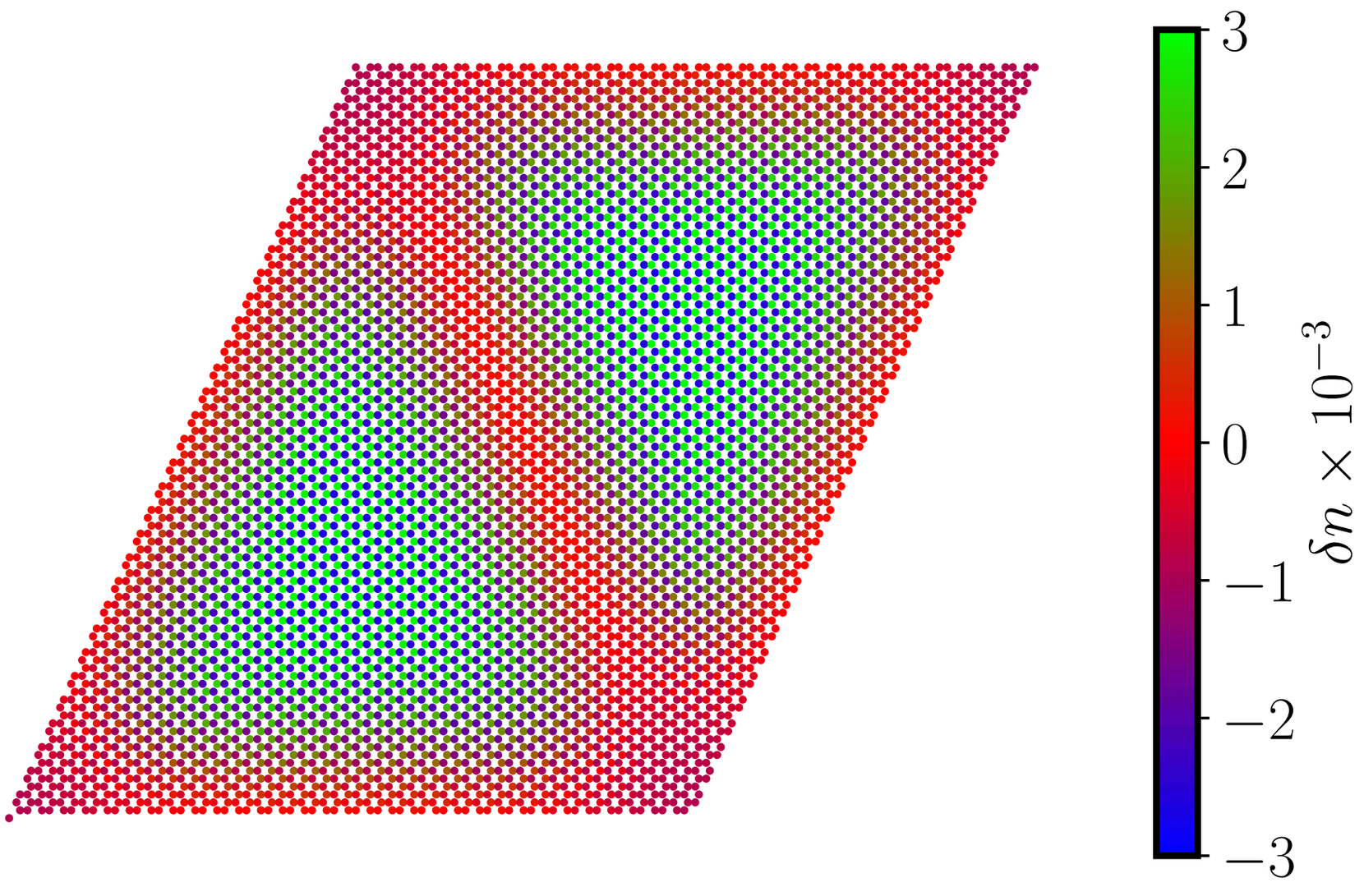
band structure of hole doped tBLG



Goodwin et al., arXiv:2004.14784

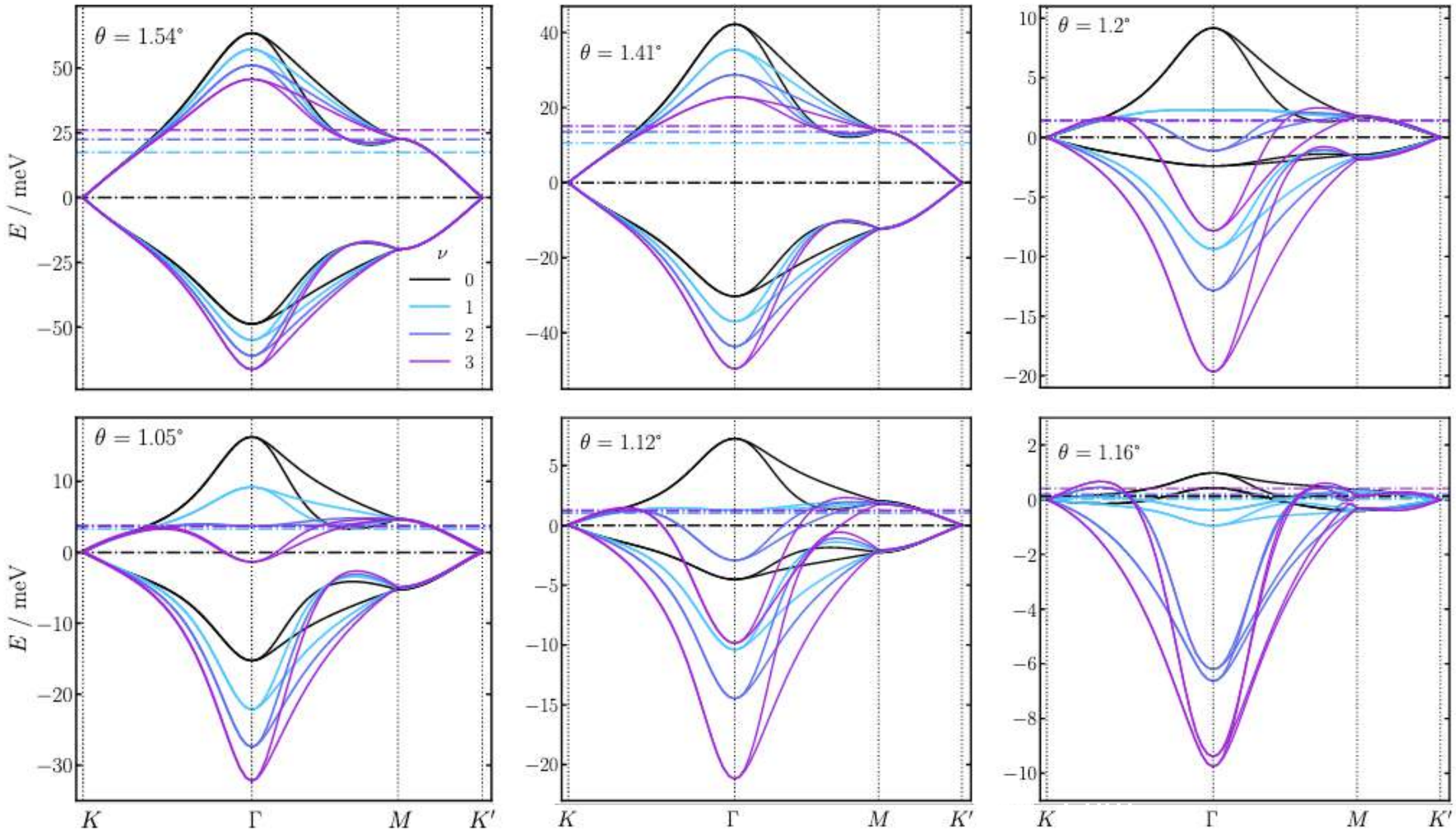
UNDERSTANDING THE NORMAL STATE

charge density of doped tBLG



UNDERSTANDING THE NORMAL STATE

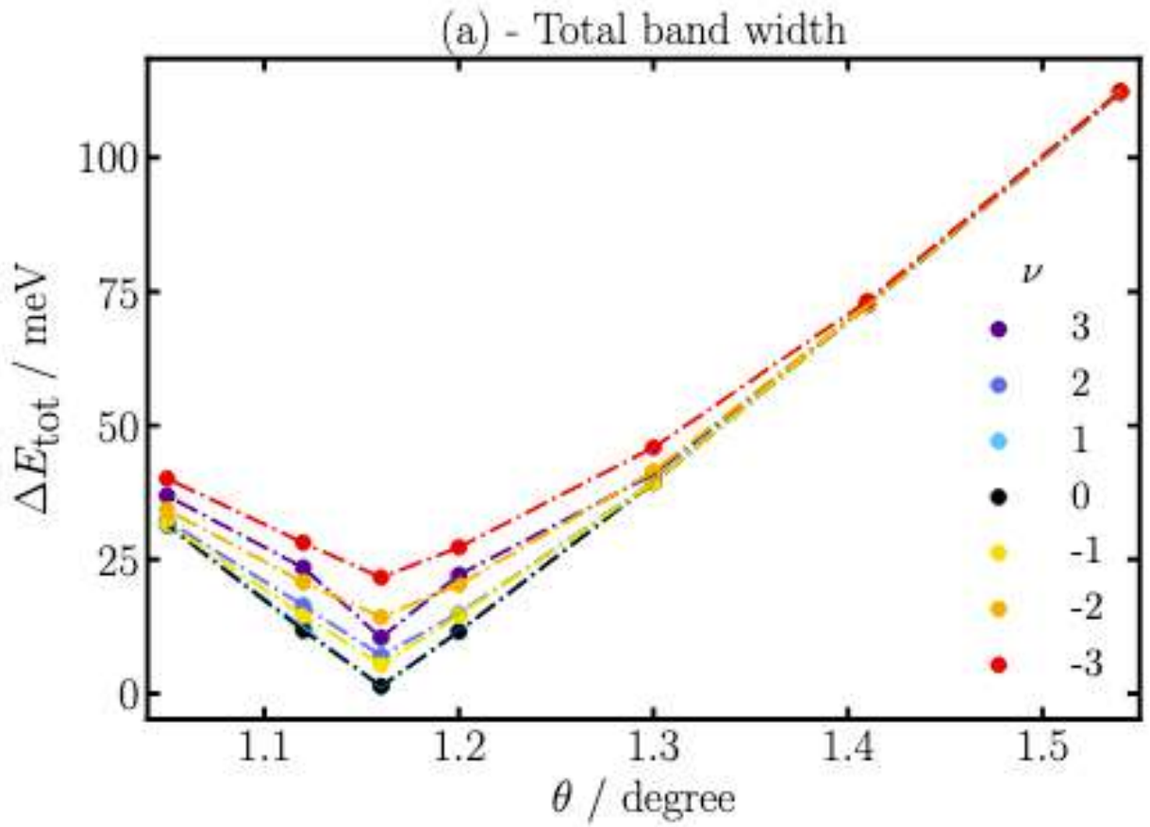
electron doped band structure as function of twist angle

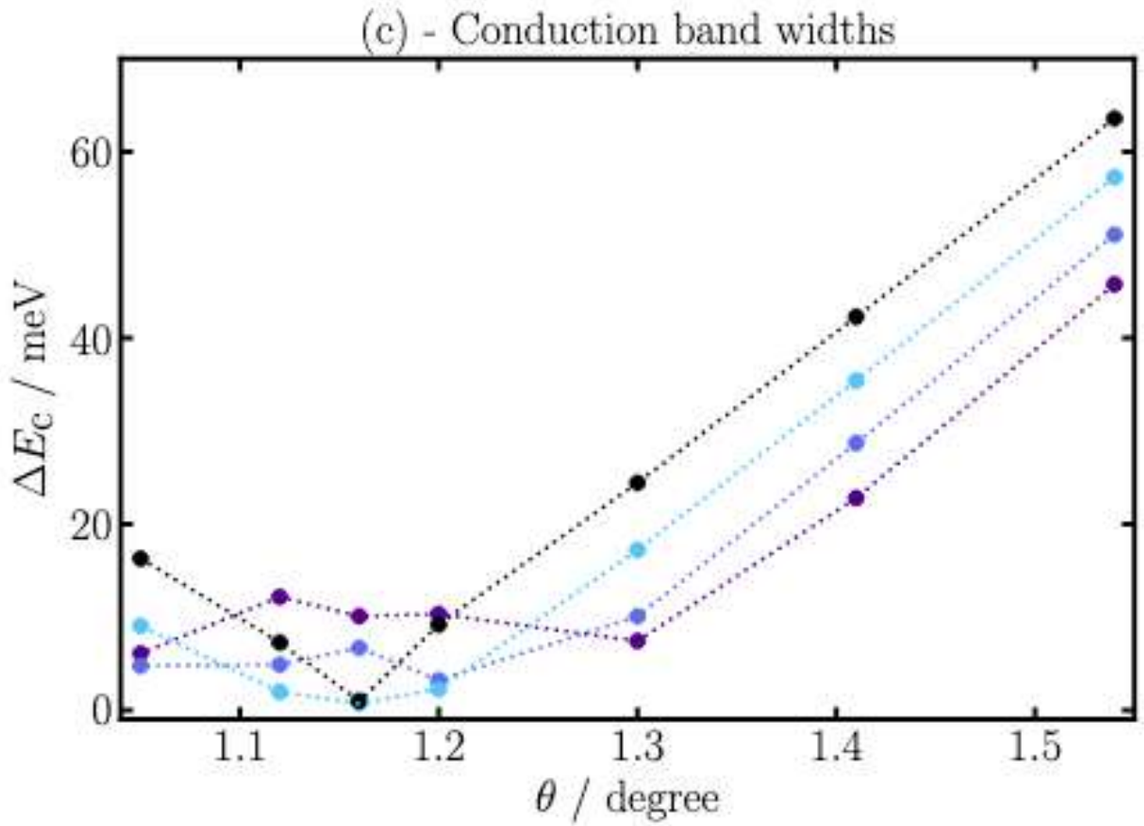


Goodwin et al., arXiv:2004.14784

UNDERSTANDING THE NORMAL STATE

How to define the magic angle?

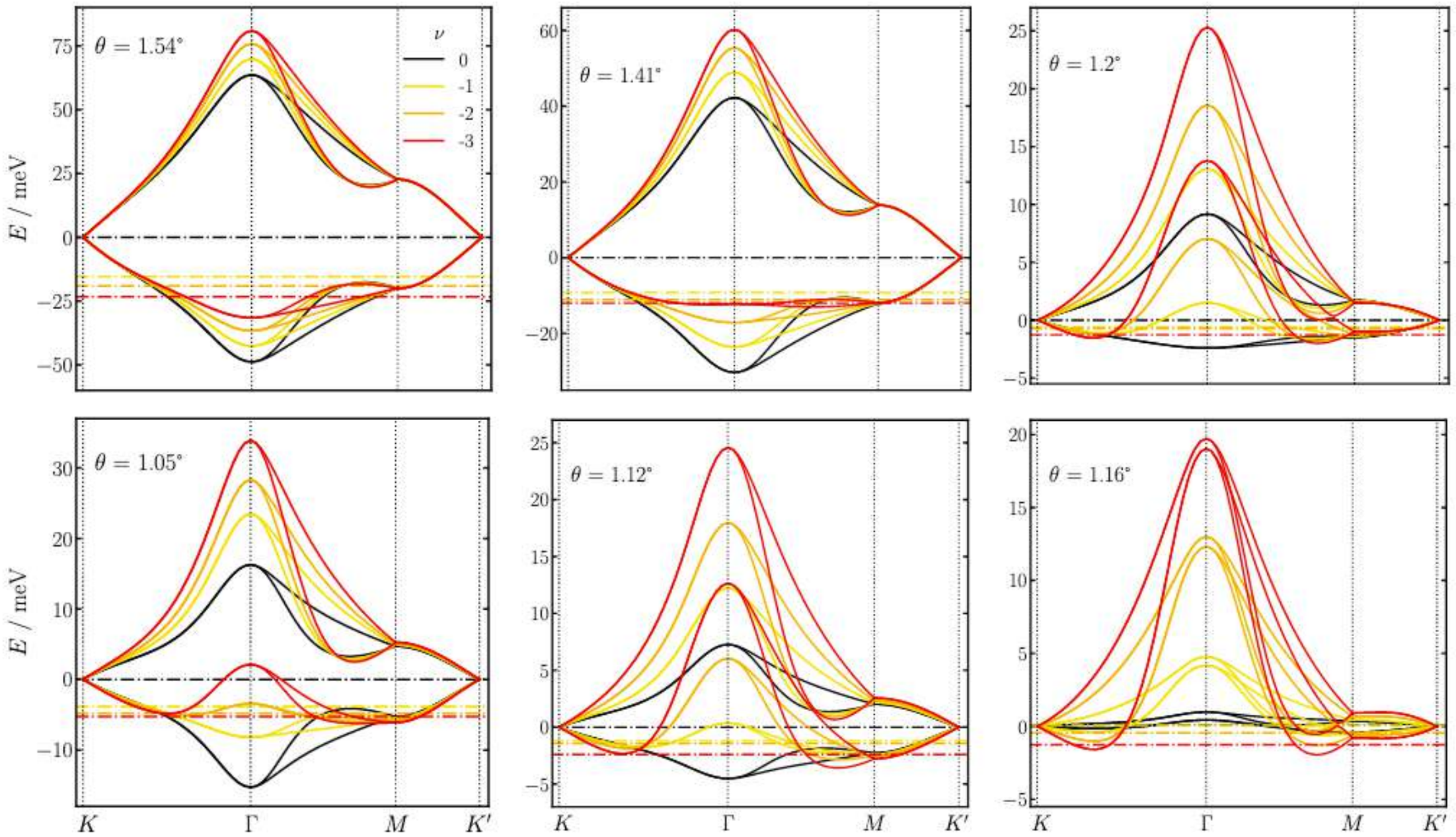




Goodwin et al., arXiv:2004.14784

UNDERSTANDING THE NORMAL STATE

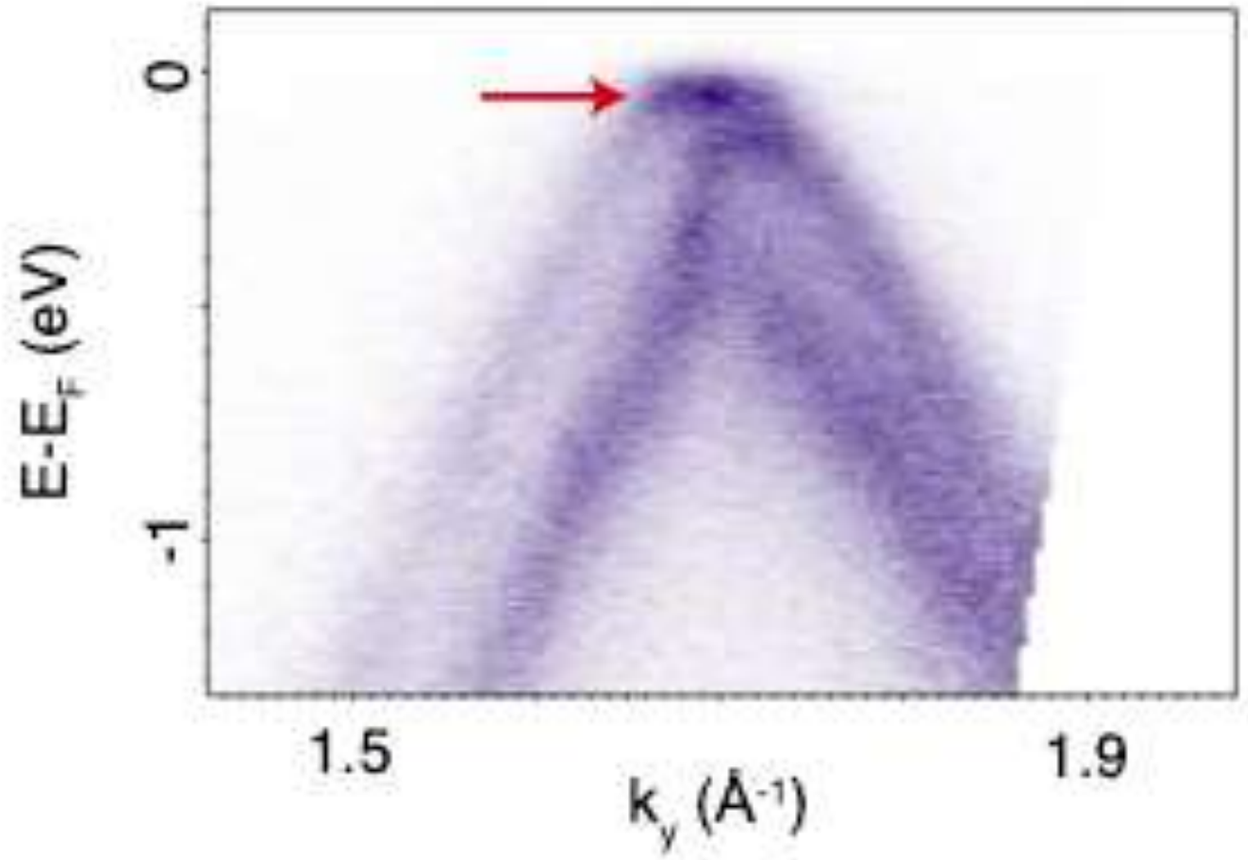
band structure of hole doped tBLG as function of twisted angle



Goodwin et al., arXiv:2004.14784

UNDERSTANDING THE NORMAL STATE

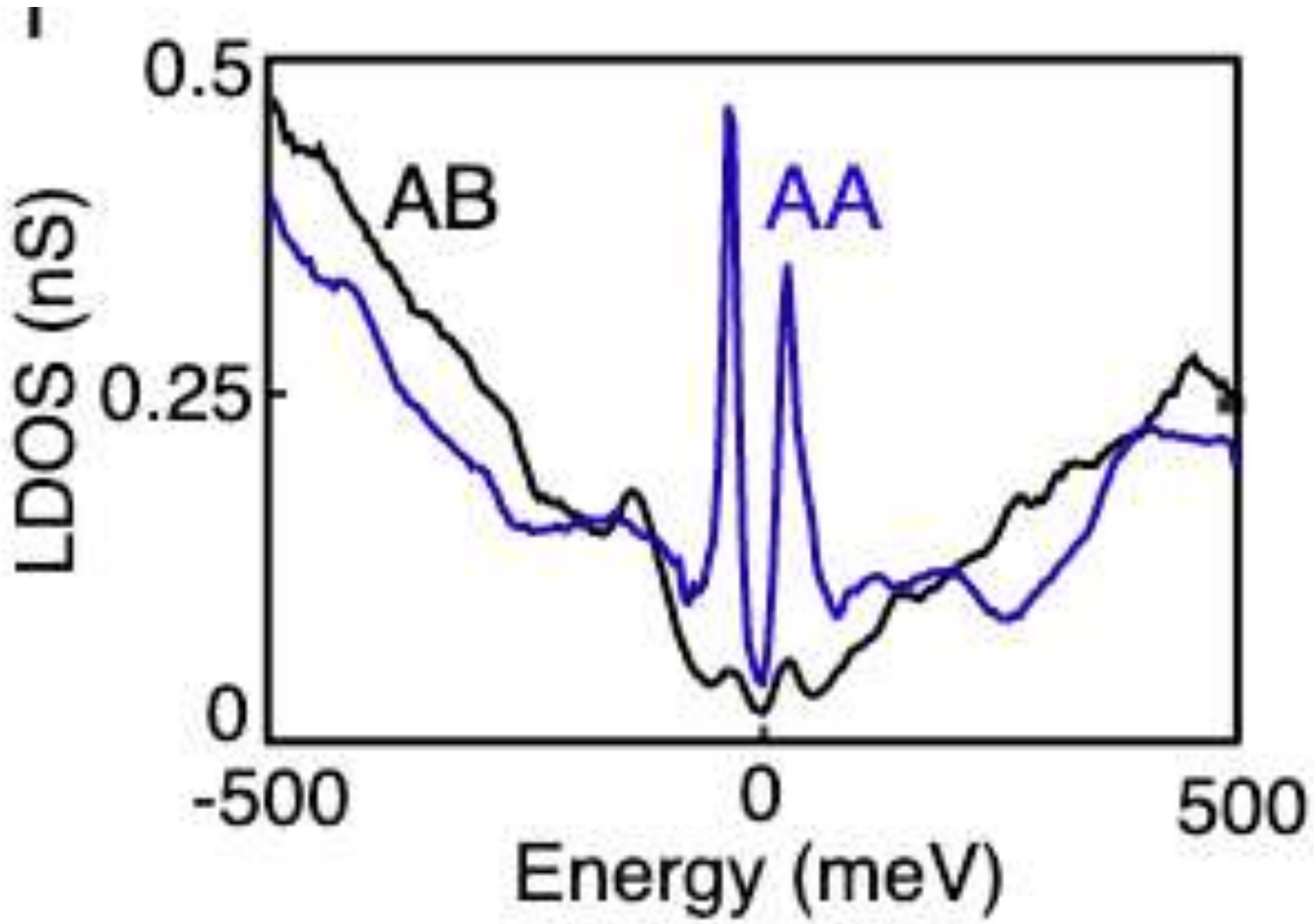
comparison to experiment: nano-ARPES



Lisi et al., arXiv:2002.02289

UNDERSTANDING THE NORMAL STATE

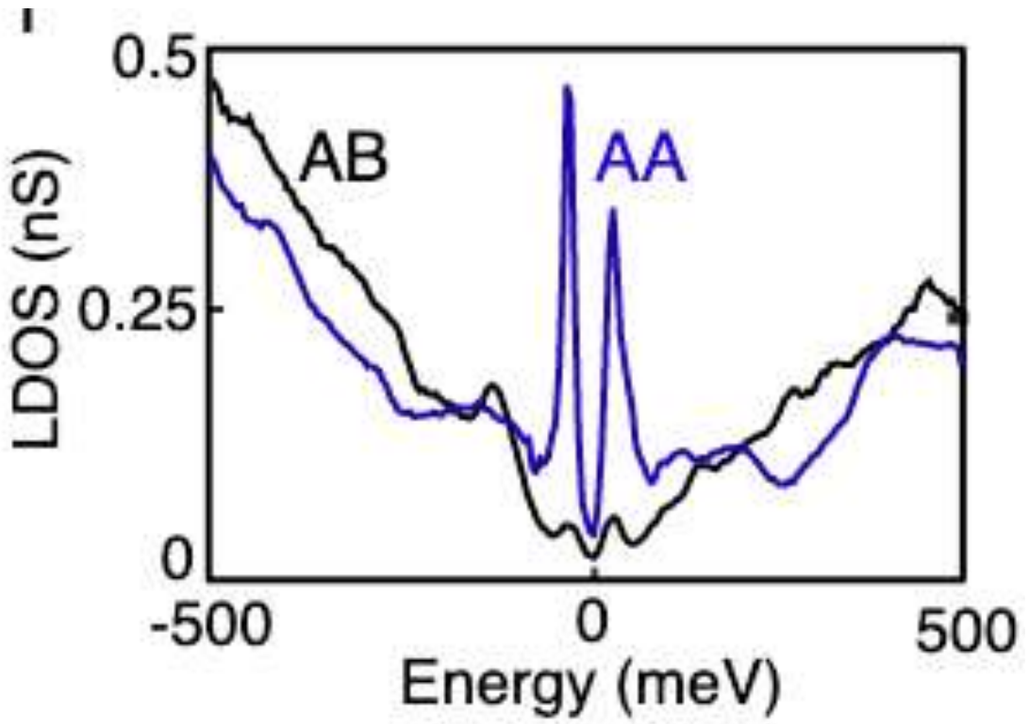
comparison to experiment: STM

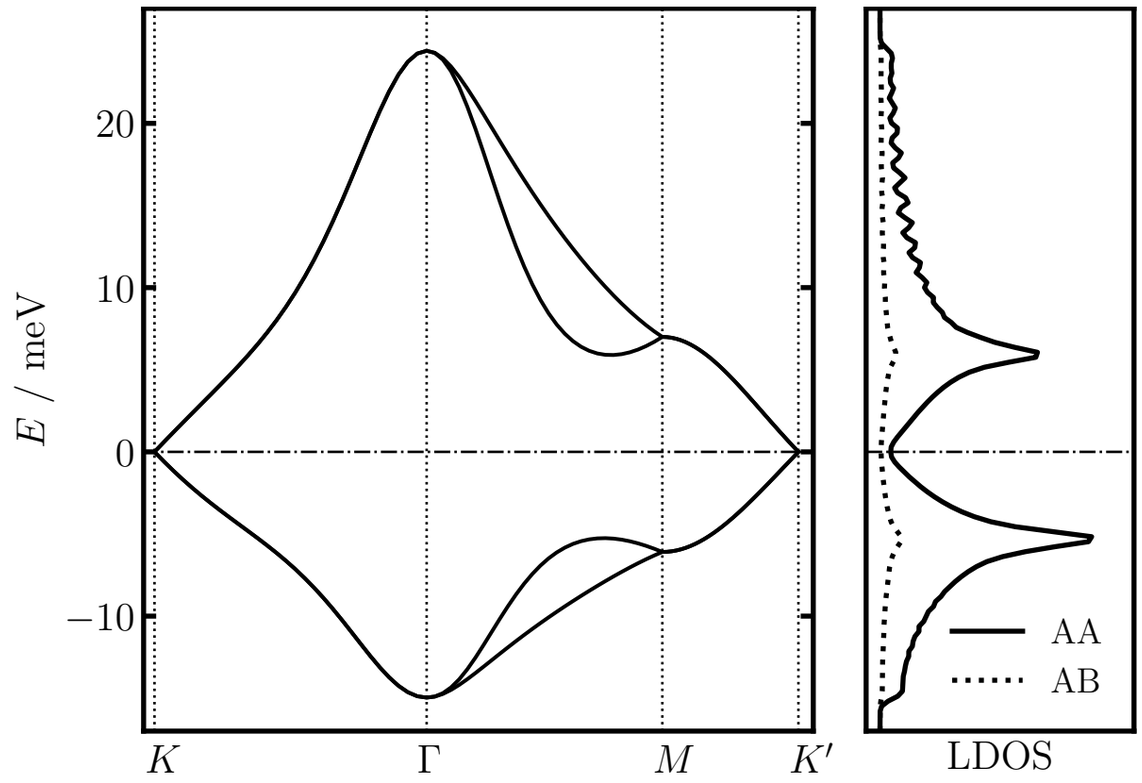


Kerelsky et al., Nature 572, 95 (2019)

UNDERSTANDING THE NORMAL STATE

comparison to experiment: STM

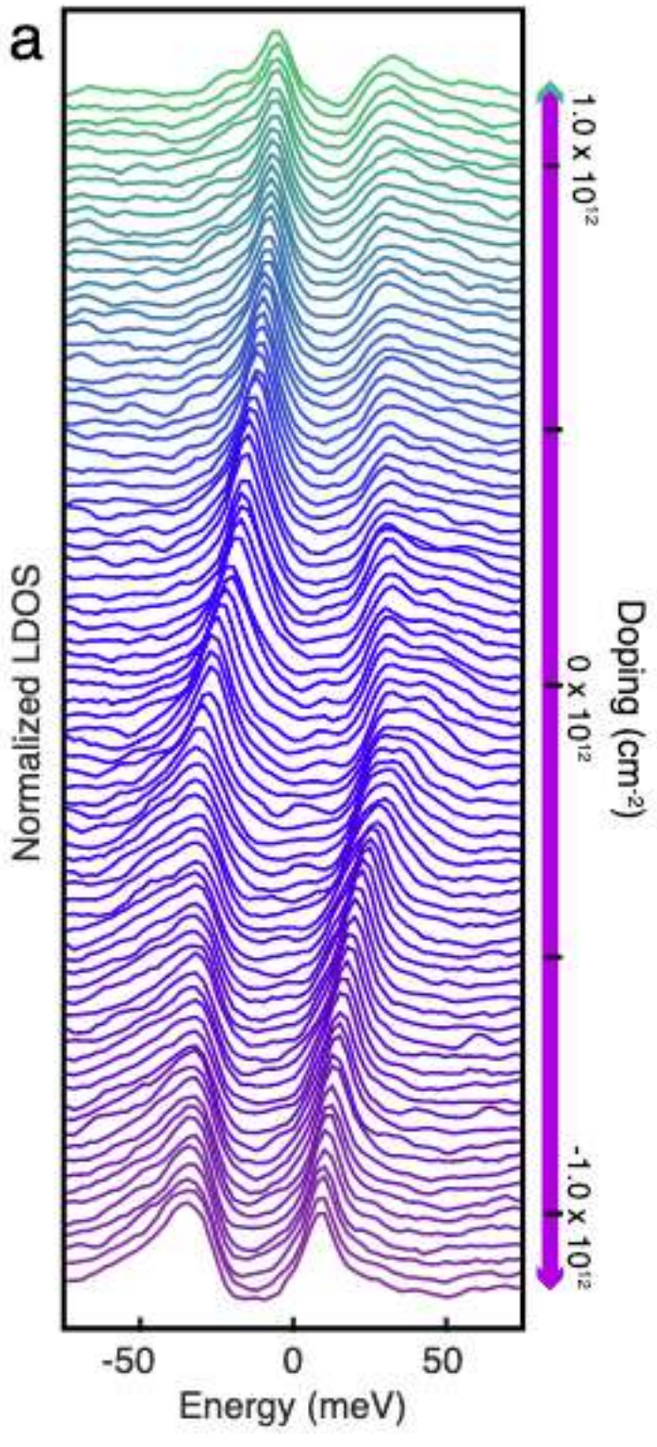


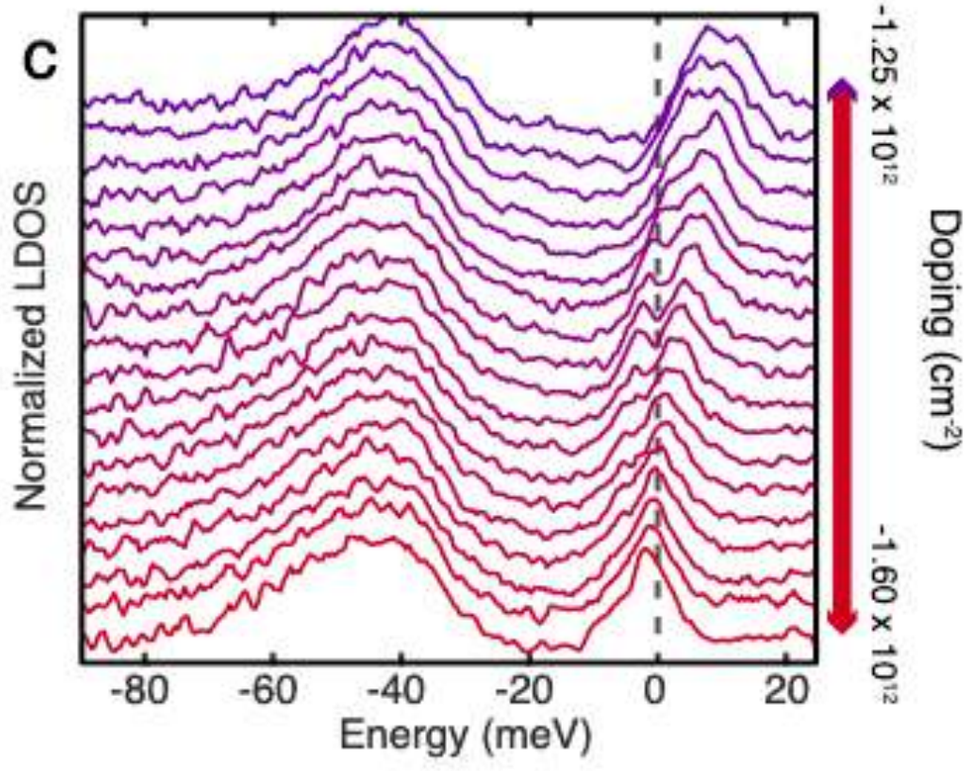


Kerelsky et al., Nature 572, 95 (2019)

UNDERSTANDING THE NORMAL STATE

STM: evolution as spectrum as function of doping

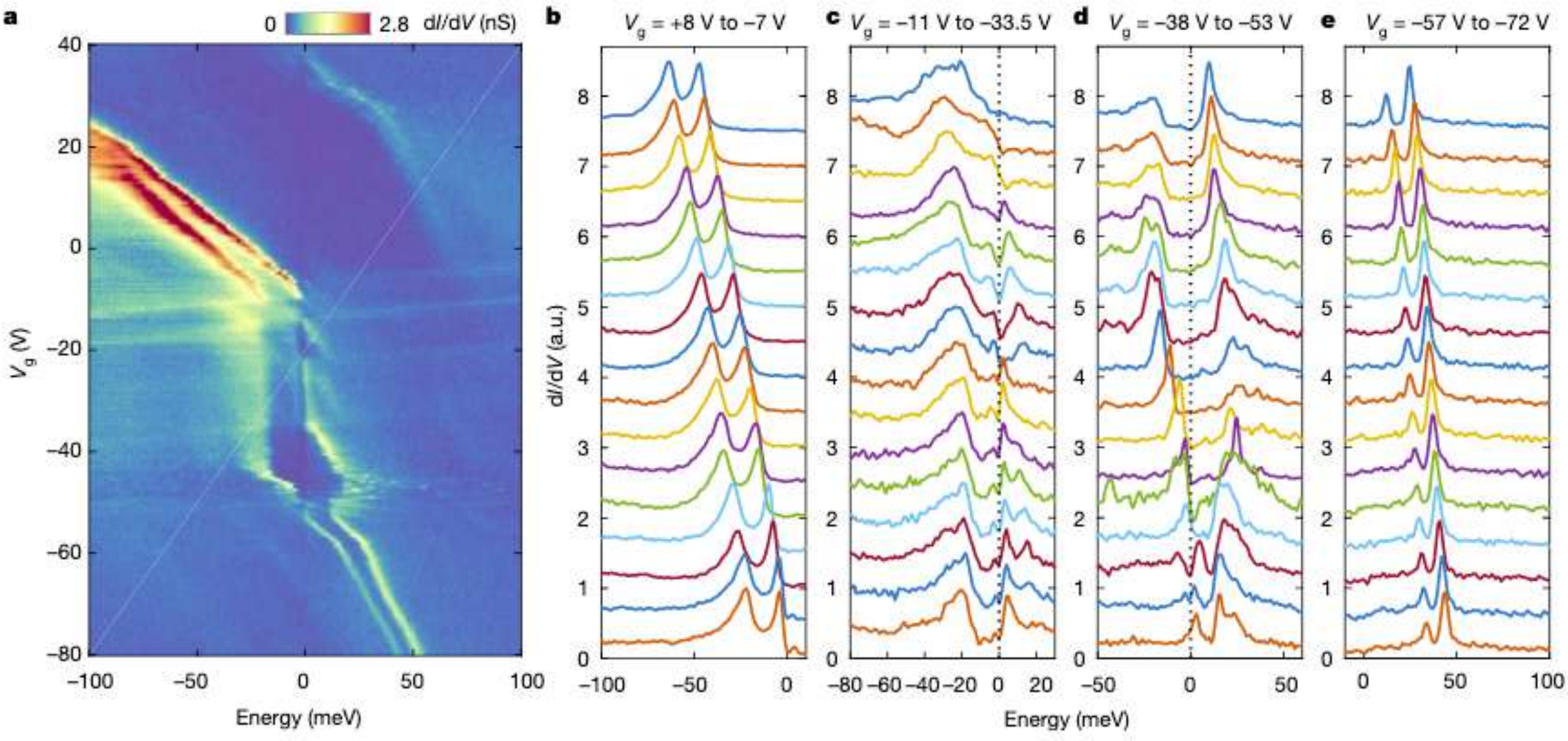




Kerelsky et al., Nature 572, 95 (2019)

UNDERSTANDING THE NORMAL STATE

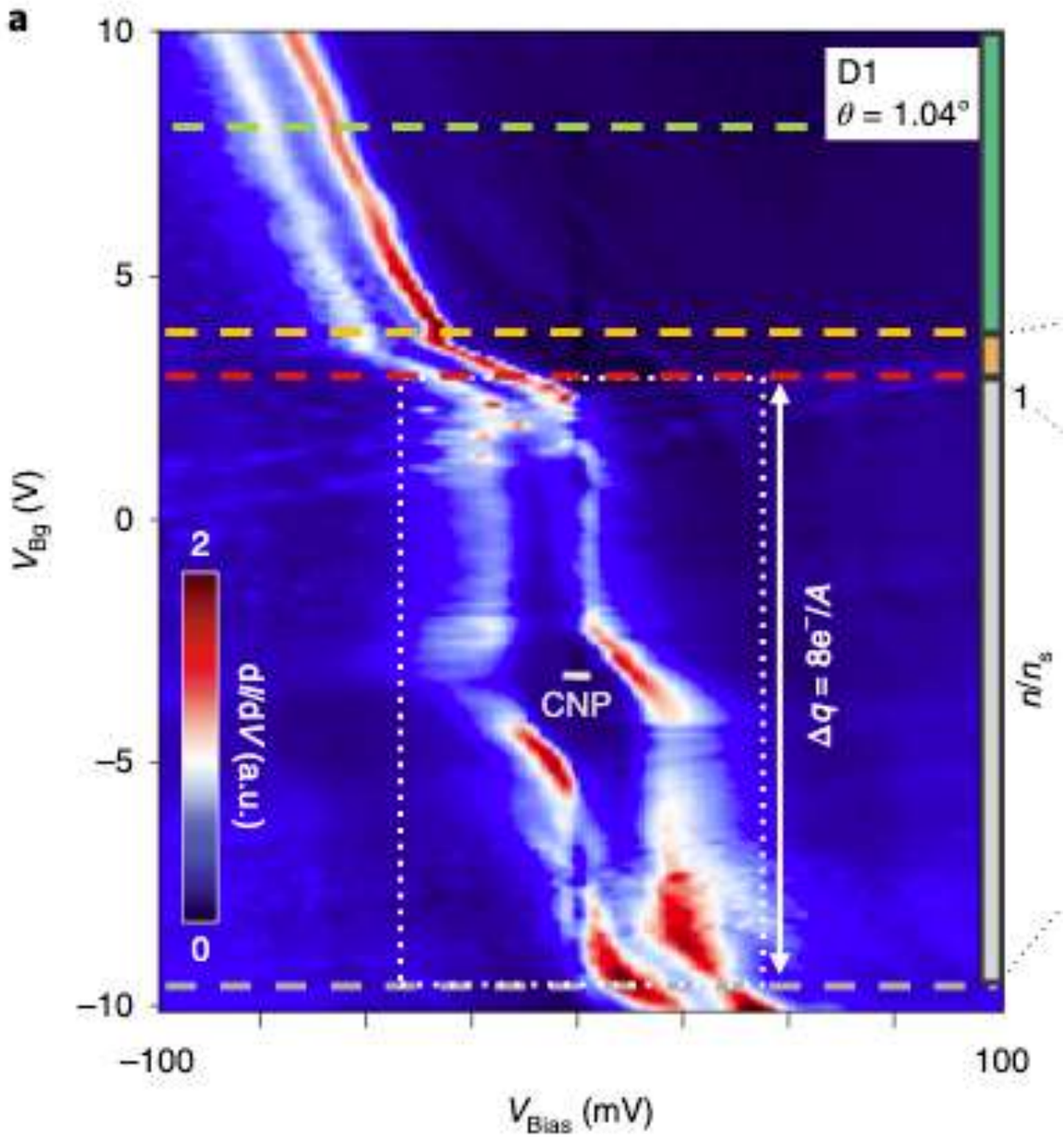
STM: evolution as spectrum as function of doping



Xie et al., Nature 572, 101 (2019)

UNDERSTANDING THE NORMAL STATE

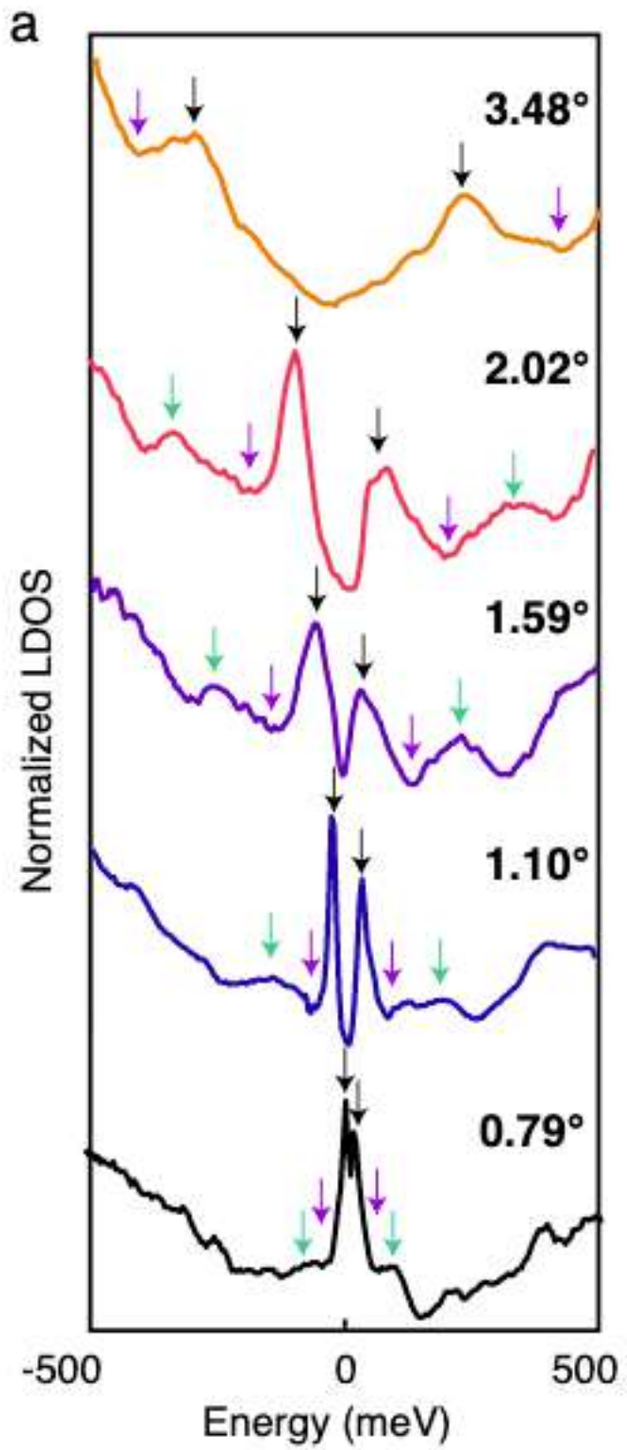
STM: evolution as spectrum as function of doping



Choi et al., Nat. Phys. 15, 174 (2019)

UNDERSTANDING THE NORMAL STATE

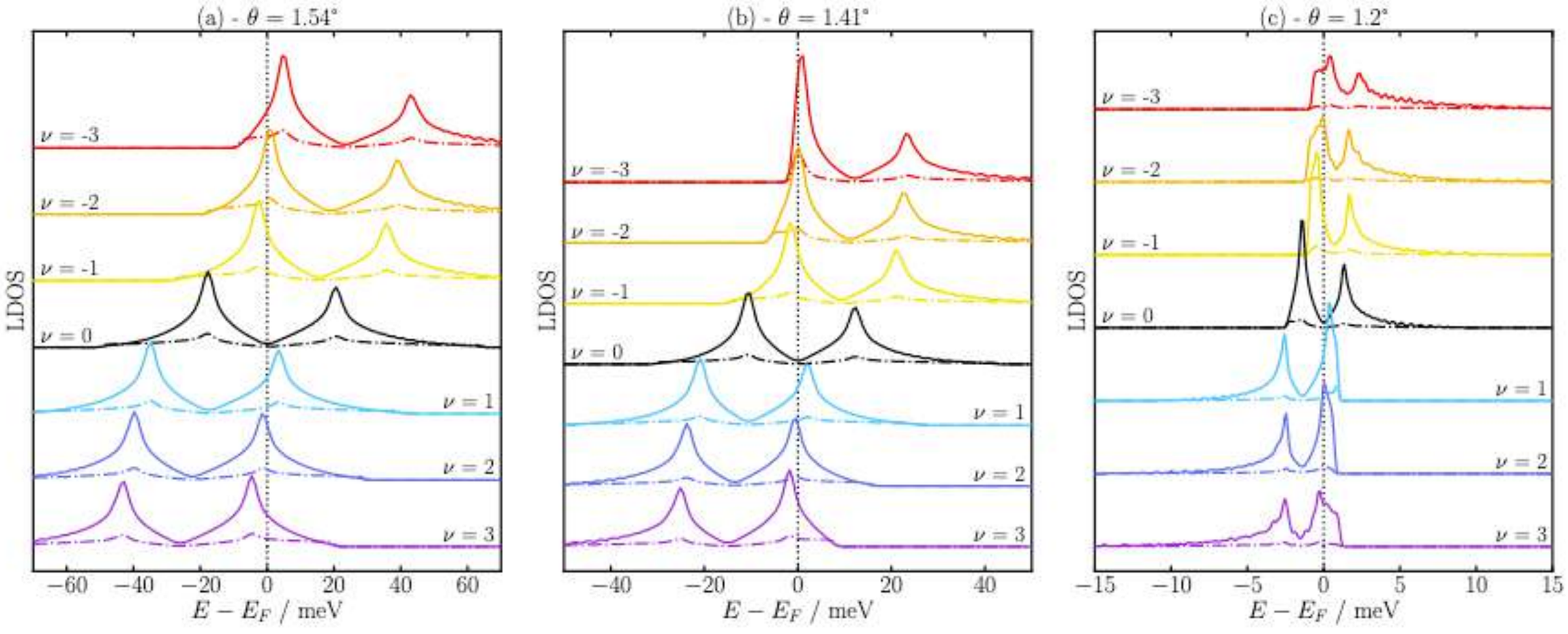
STM: evolution as spectrum as function of twist angle



Kerelsky et al., Nature 572, 95 (2019)

UNDERSTANDING THE NORMAL STATE

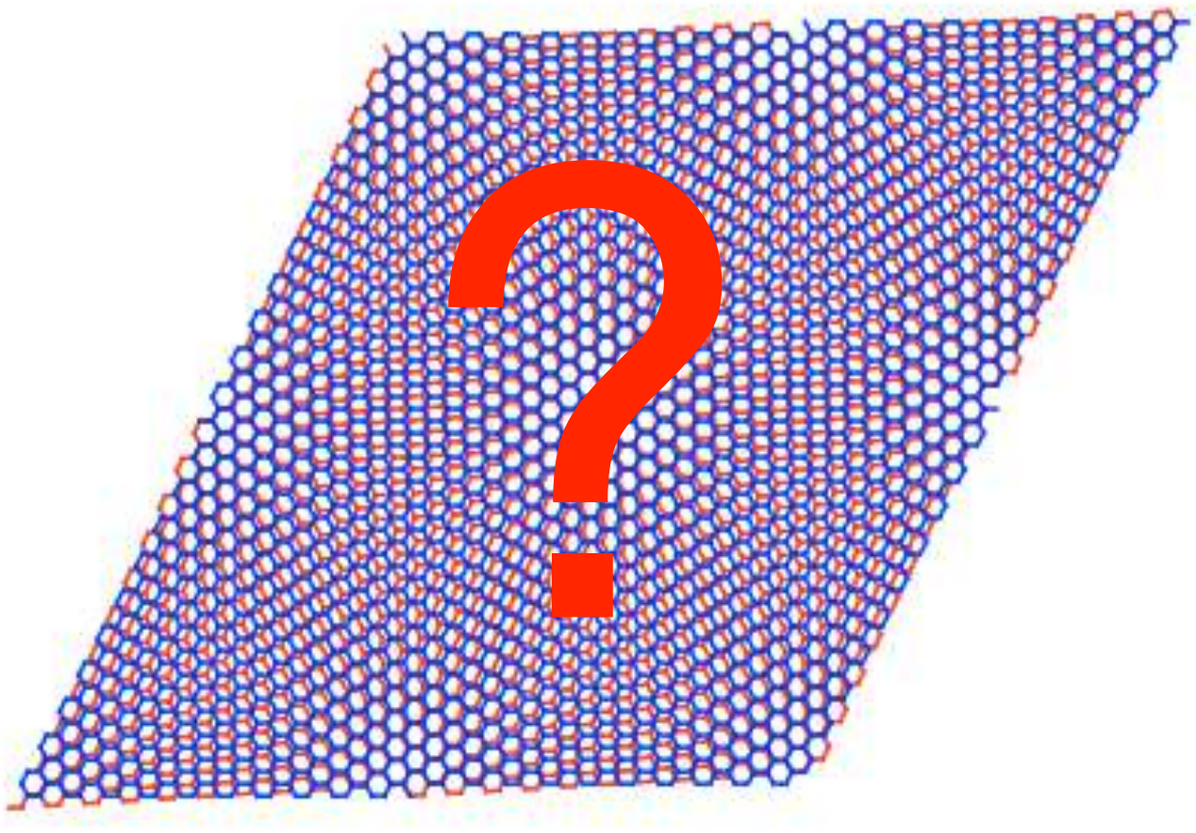
Local density of states from atomistic Hartree theory



Goodwin et al., arXiv:2004.14784

UNDERSTANDING MOIRE MATERIALS

What is the role of electron-electron interactions?



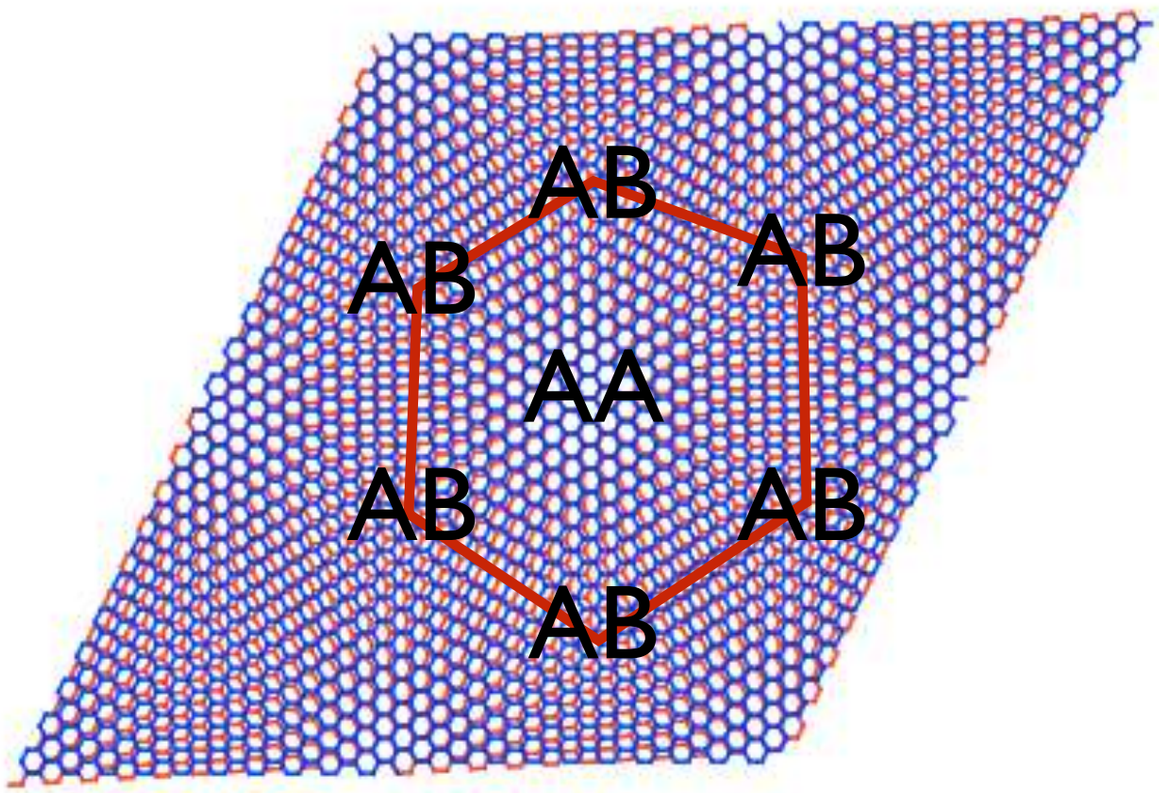
UNDERSTANDING MOIRE MATERIALS

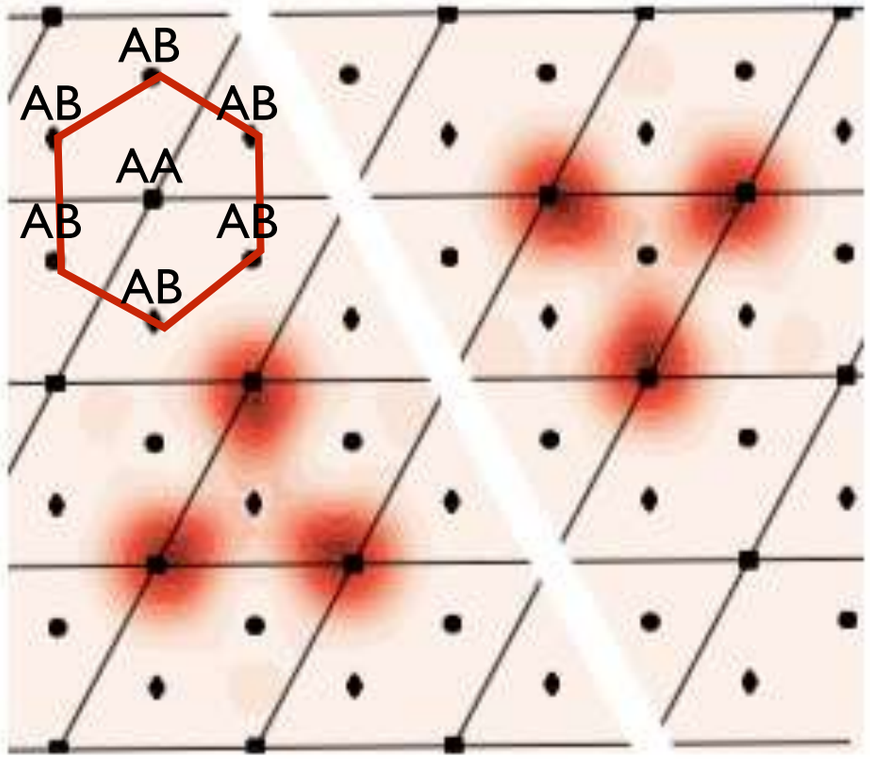
Broken symmetry states and Hubbard Hamiltonian

$$H = t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

What is U/t in twisted bilayer graphene?

WANNIER FUNCTIONS



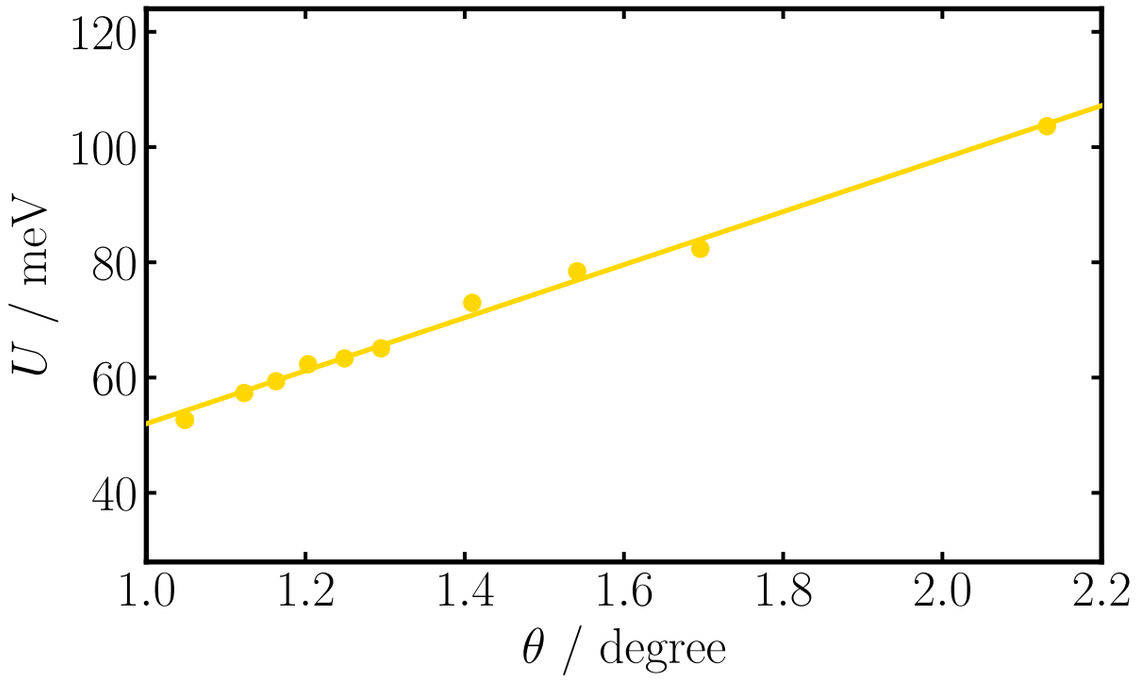


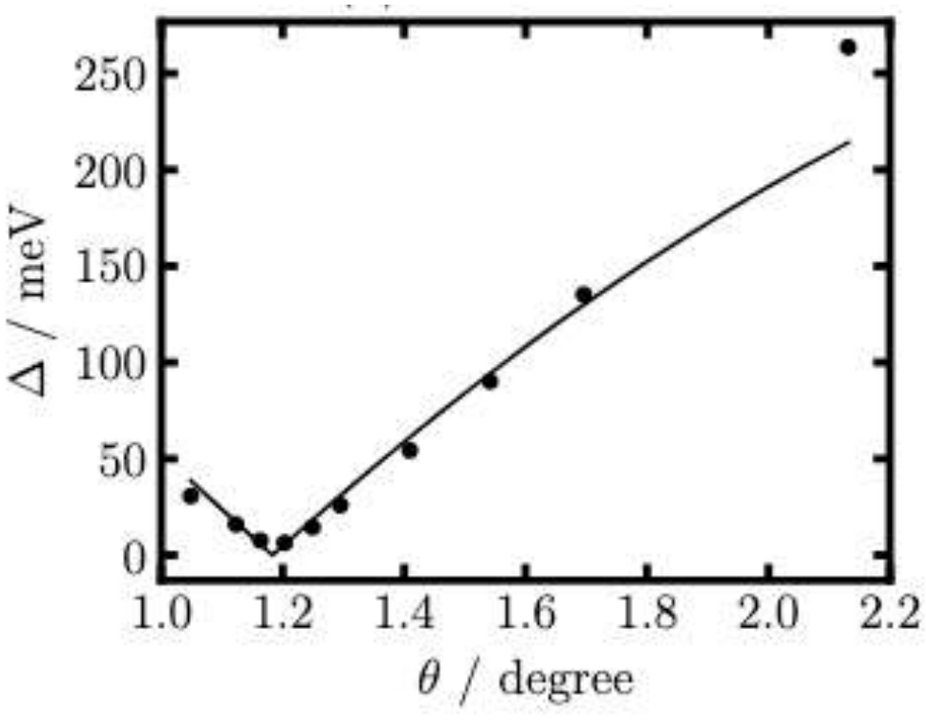
$$t = \langle w_{n\mathbf{R}'} | H_{DFT} | w_{n\mathbf{R}} \rangle$$

$$U = \langle w_{n\mathbf{R}} w_{n\mathbf{R}} | W | w_{n\mathbf{R}} w_{n\mathbf{R}} \rangle$$

Goodwin et al., Phys. Rev. B 100, 121106 (2019)

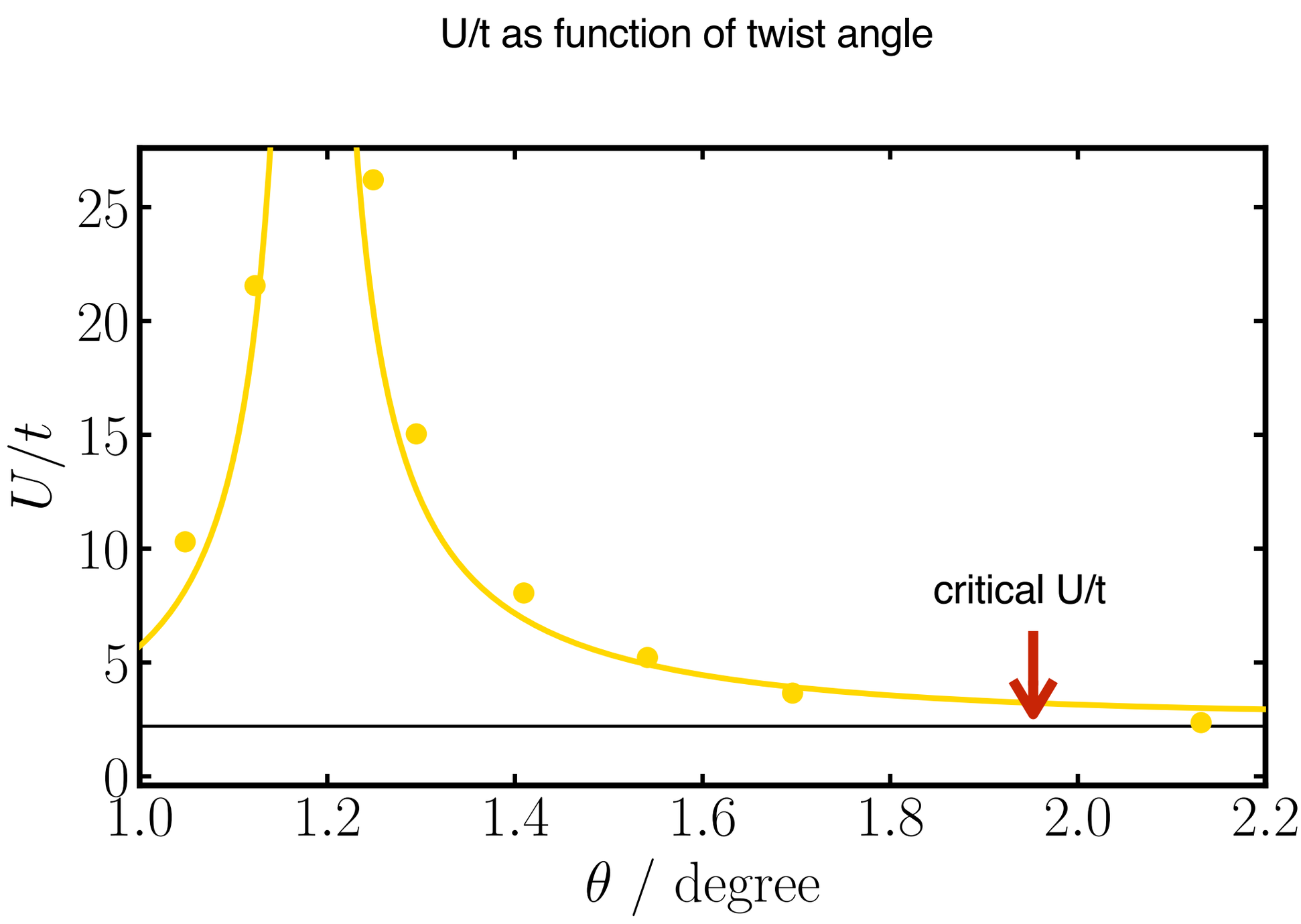
PARAMETERS OF HUBBARD HAMILTONIAN





Goodwin et al., Phys. Rev. B 100, 121106 (2019)

THE STRENGTH OF ELECTRON CORRELATIONS



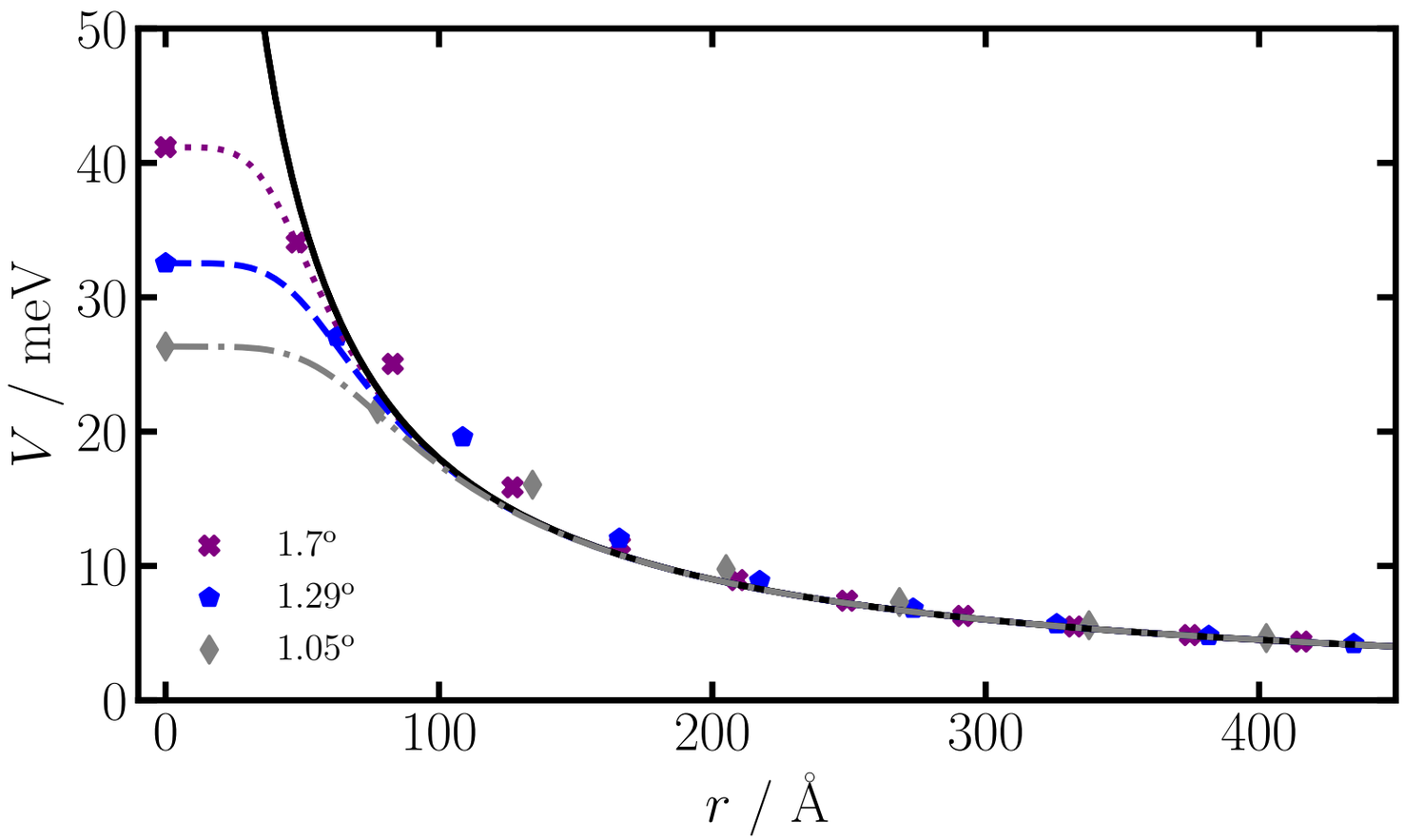
Goodwin et al., Phys. Rev. B 100, 121106 (2019)

LONG RANGED INTERACTIONS

Extended Hubbard interactions

$$V_{ij} = \iint d\mathbf{r} d\mathbf{r}' |w_i(\mathbf{r})|^2 W(\mathbf{r}-\mathbf{r}') |w_j(\mathbf{r}')|^2.$$

$$W(\mathbf{r}-\mathbf{r}') = \frac{e^2}{4\pi\epsilon_0\epsilon_r|\mathbf{r}-\mathbf{r}'|}$$

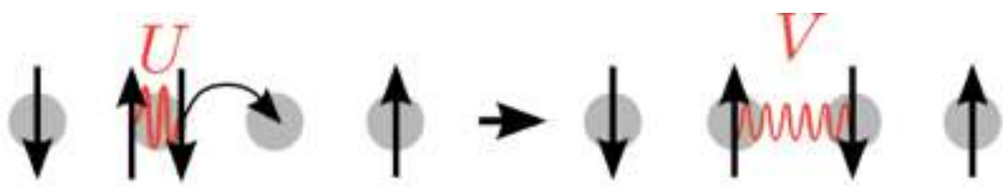


Goodwin et al., Phys. Rev. B 100, 121106 (2019)

LONG RANGED INTERACTIONS

Mapping onto short-ranged Hubbard model

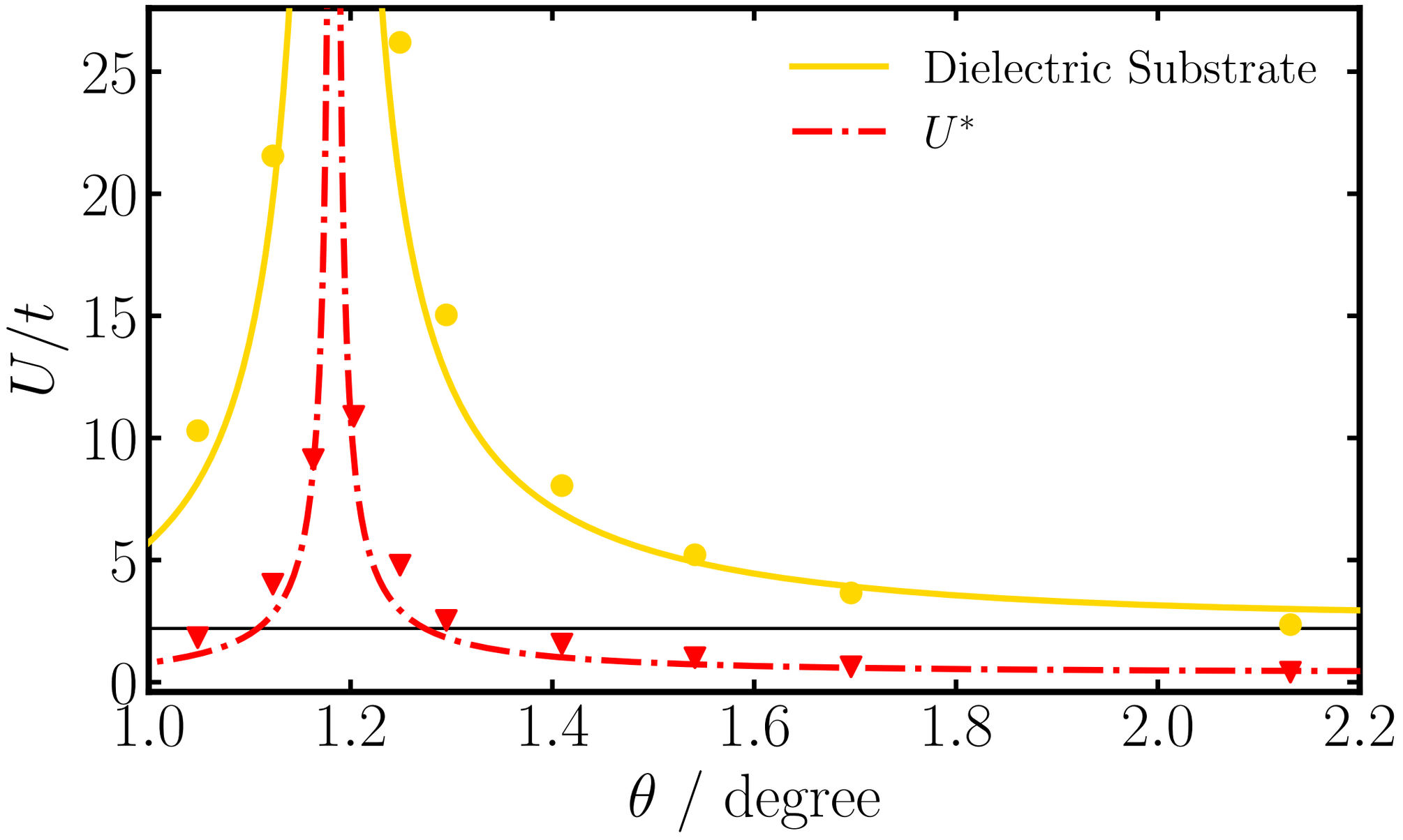
$$U^* = V_{00} - V_{01}$$



Schueler et al., Phys. Rev. Lett. 111, 036601 (2013)

LONG RANGED INTERACTIONS

U/t as function of twist angle



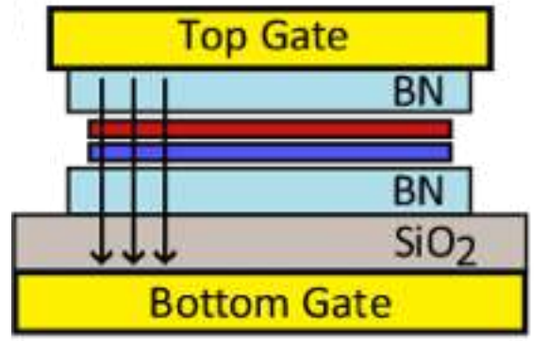
Goodwin et al., Phys. Rev. B 100, 121106 (2019)

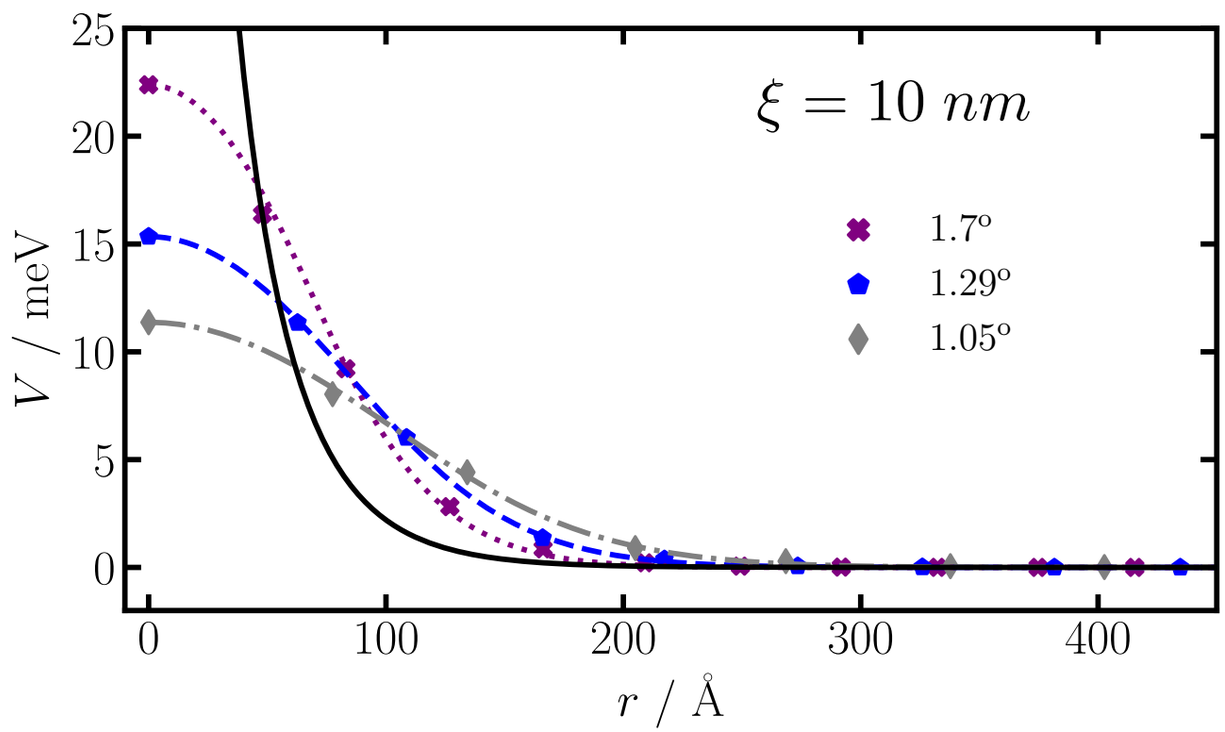
SCREENING

External

$$V_{ij} = \iint d\mathbf{r}d\mathbf{r}'|w_i(\mathbf{r})|^2 W(\mathbf{r}-\mathbf{r}')|w_j(\mathbf{r}')|^2.$$

$$W^g(\mathbf{r}-\mathbf{r}') = \frac{e^2}{4\pi\epsilon_r\epsilon_0}\sum_{n=-\infty}^{+\infty}\frac{(-1)^n}{\sqrt{|\mathbf{r}-\mathbf{r}'|^2+(\xi n)^2}}$$

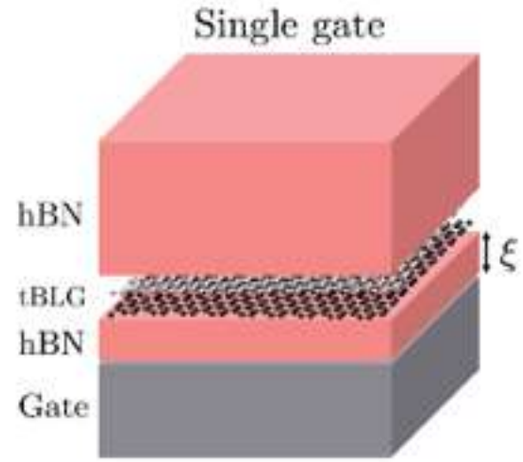


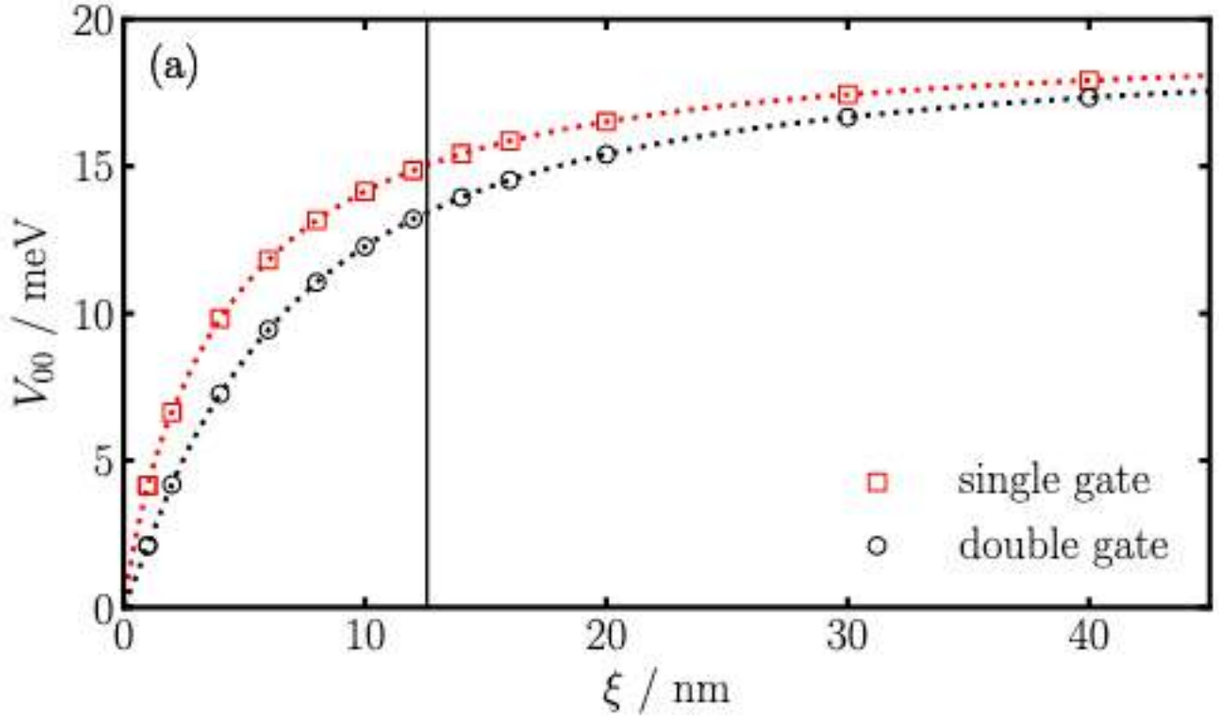


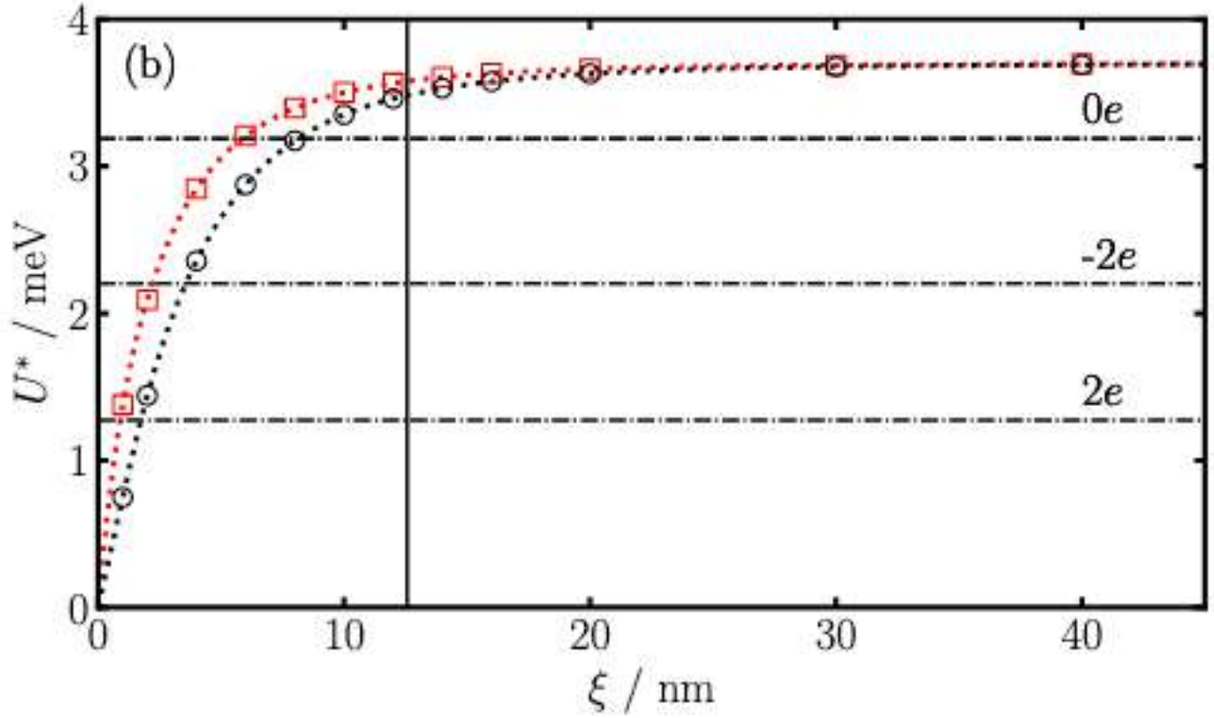
Goodwin et al., Phys. Rev. B 100, 121106 (2019)

SCREENING

Dependence on thickness of hBN layer



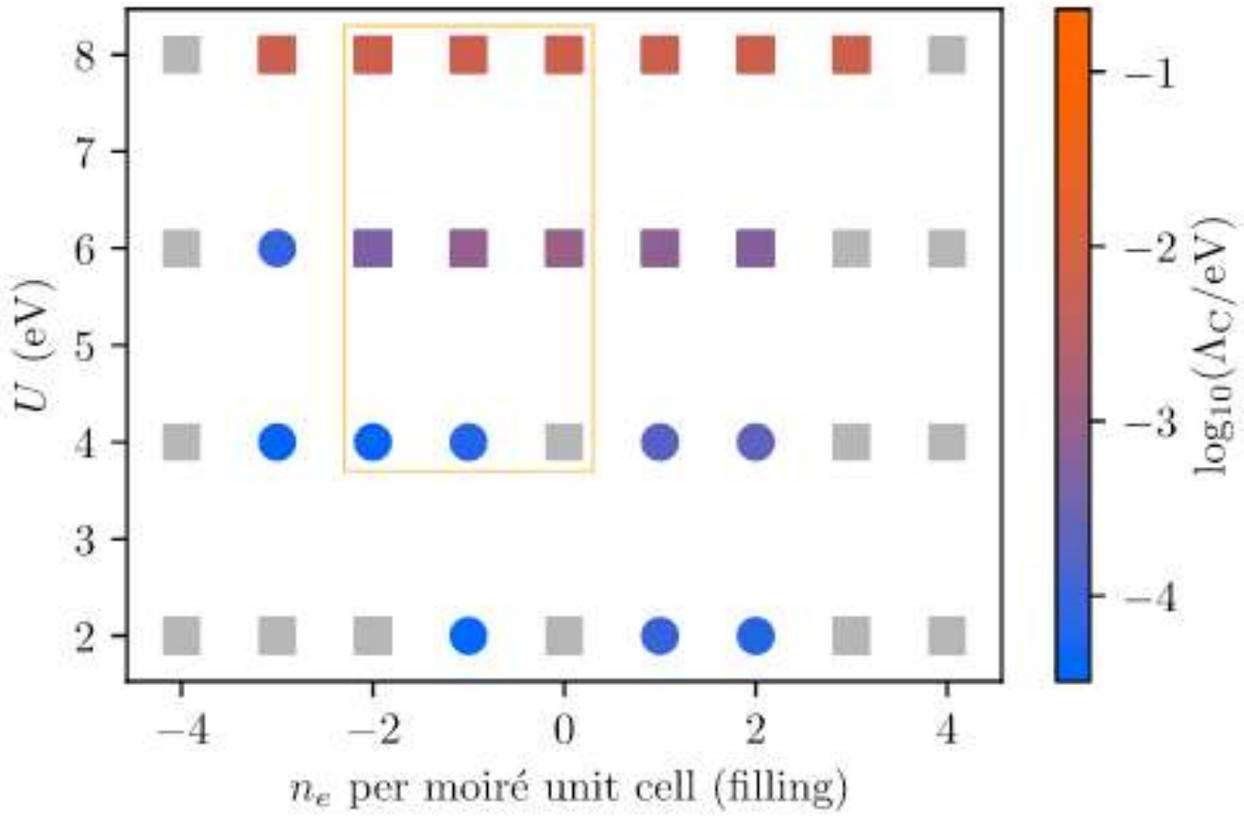


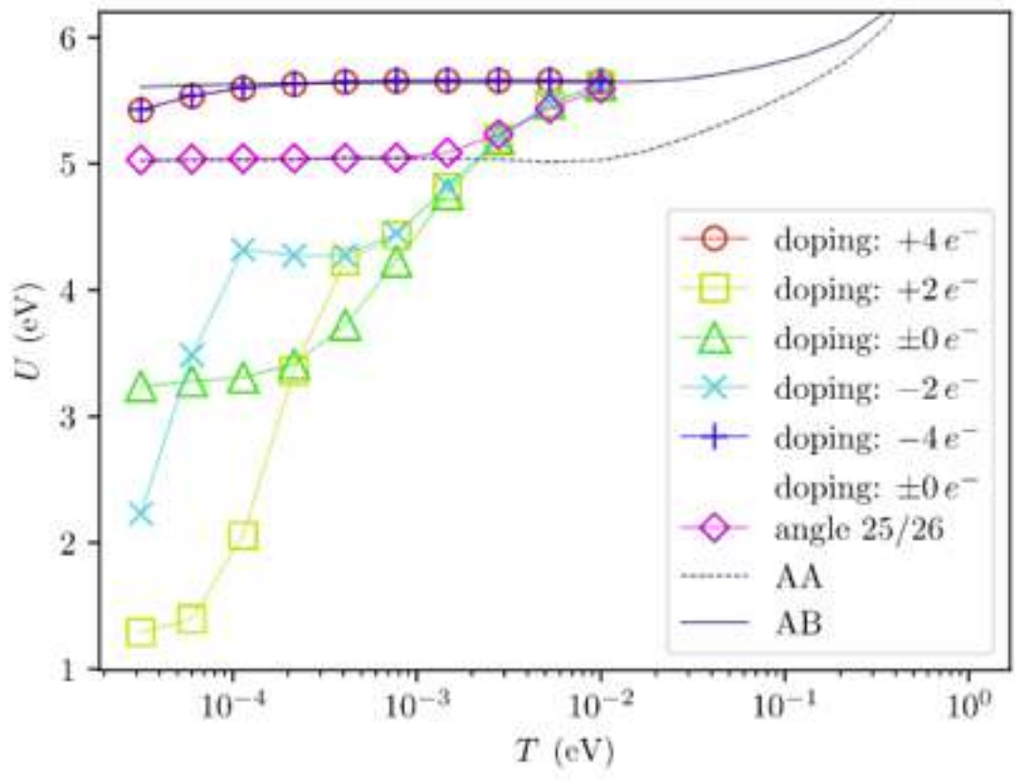


Goodwin et al., Phys. Rev. B 101, 165110 (2020)

SCREENING

Magnetic phases and critical U/t

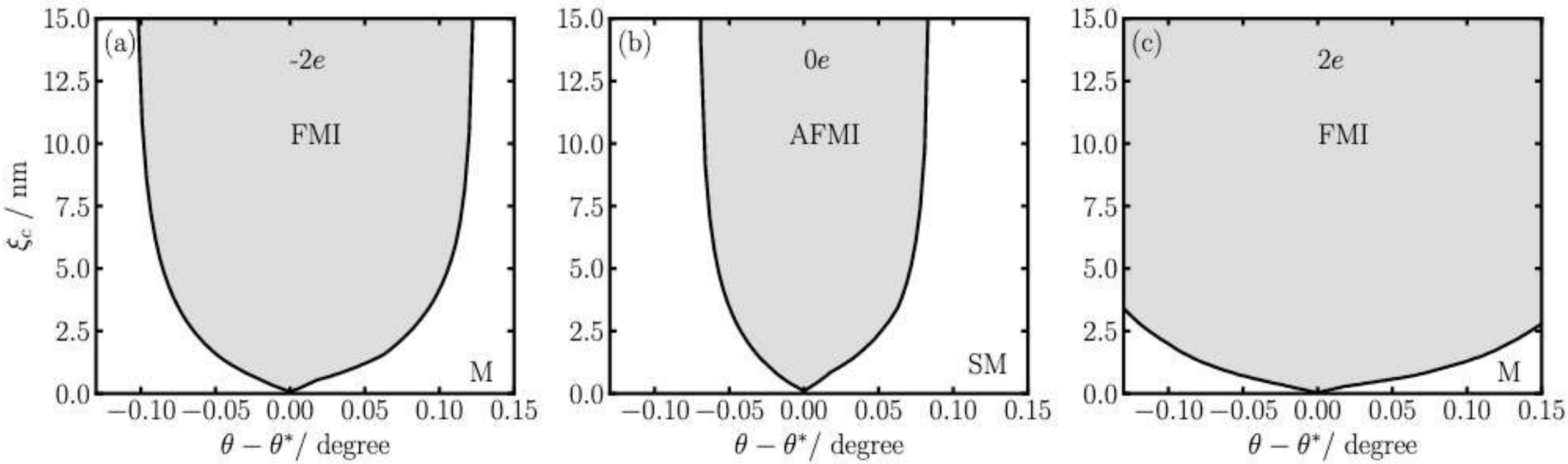




Klebl, Honerkamp, Phys. Rev. B 100, 155145 (2019)

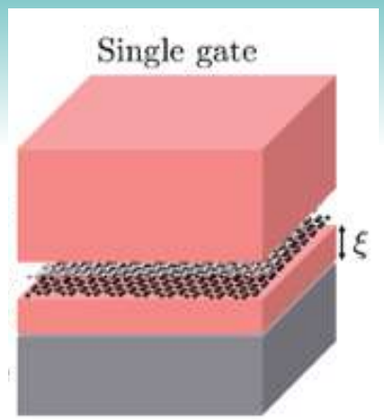
SCREENING

Phase diagrams as function of twist angle and hBN thickness

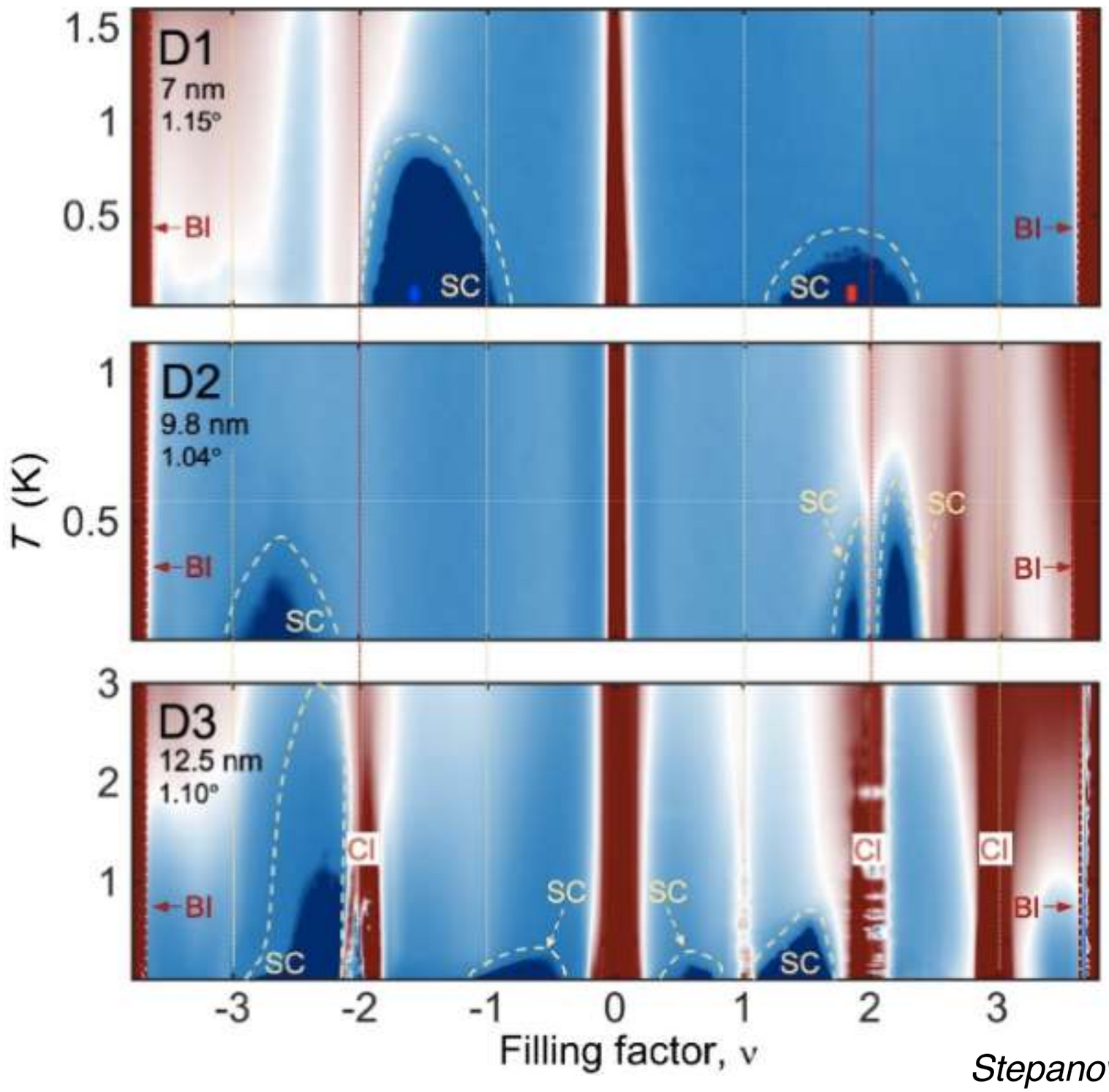


Goodwin et al., Phys. Rev. B 101, 165110 (2020)

SCREENING

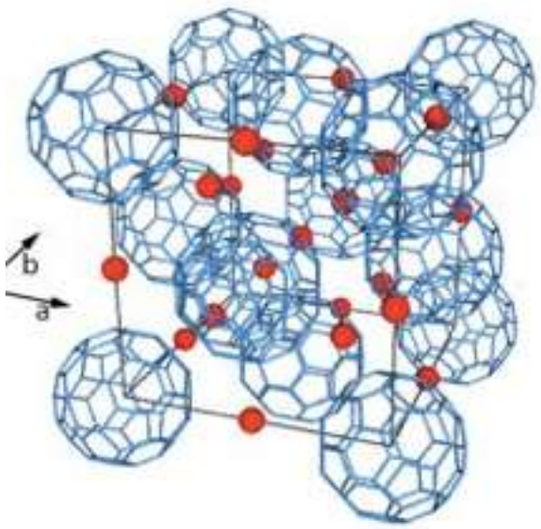


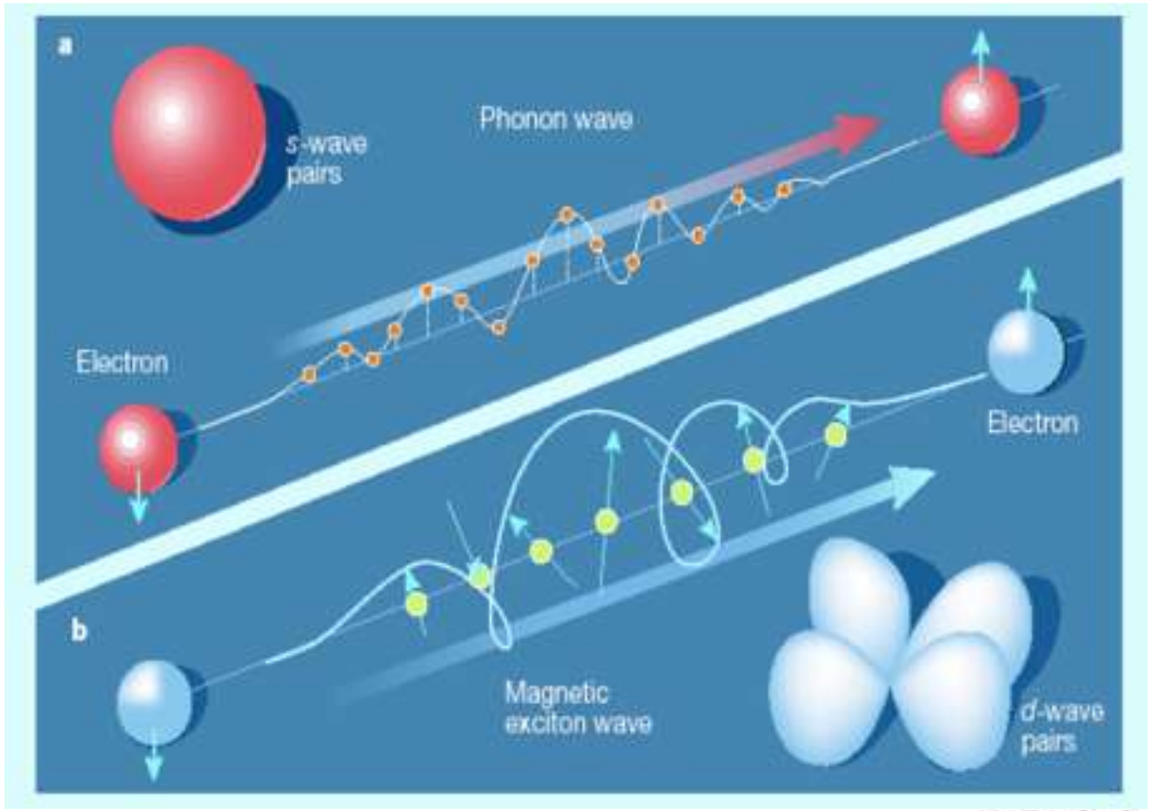
Experiment



Stepanov et al., arXiv:1911.09198

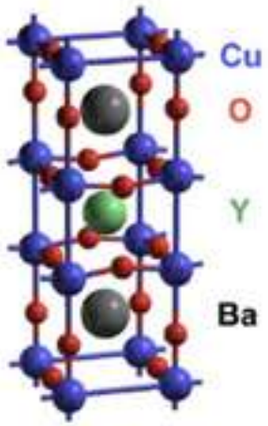
SUPERCONDUCTIVITY



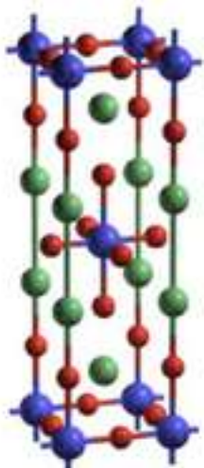


$HgBa_2CuO_{4+\delta}$ (Hg1201)

$YBa_2Cu_3O_{7-\delta}$ (YBCO)



$La_{2-x}Sr_xCuO_4$ (LSCO)

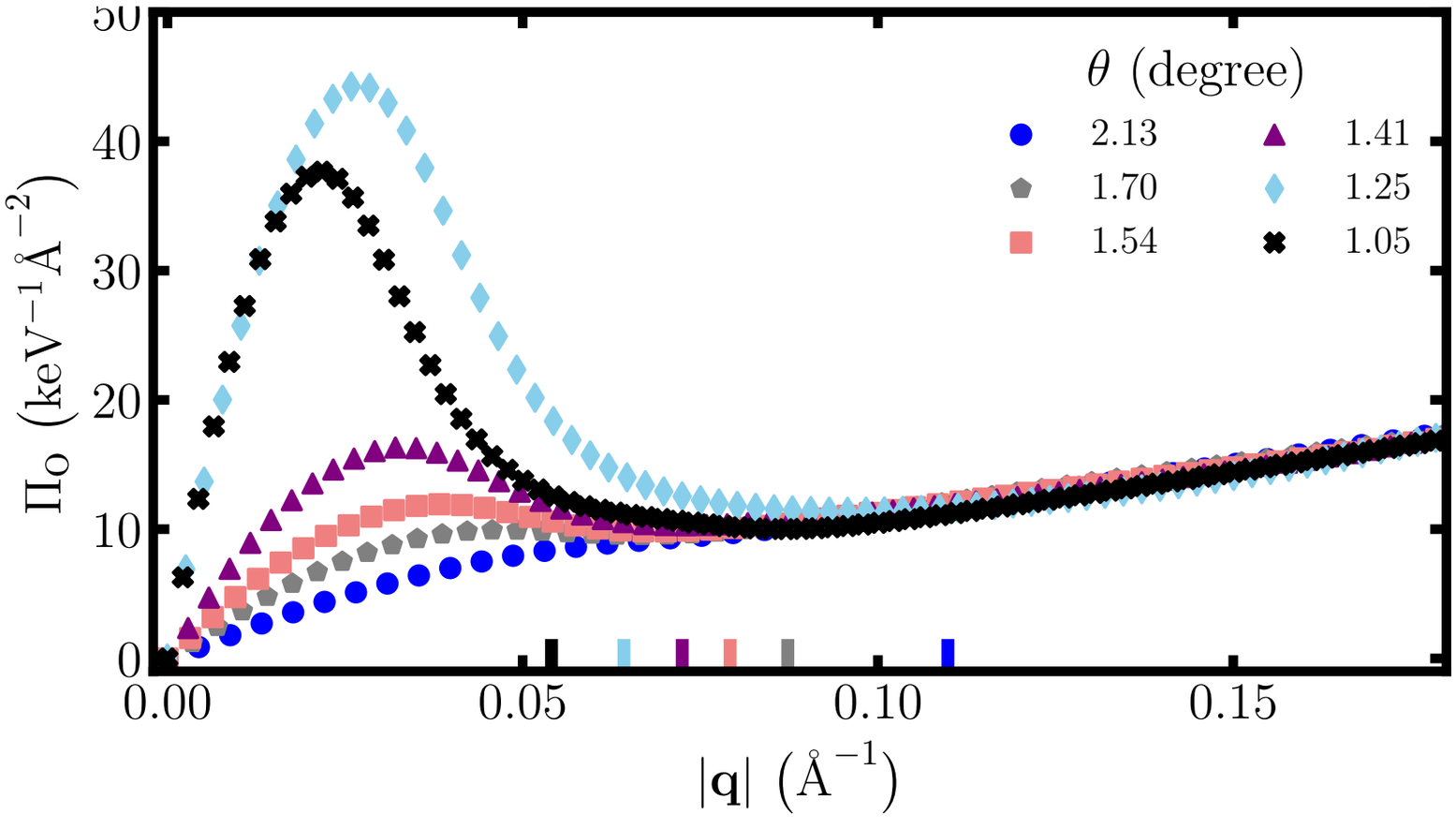


SCREENING

Internal

$$\epsilon(\mathbf{q}) = \epsilon_{env} - v(\mathbf{q})\Pi_0(\mathbf{q});$$

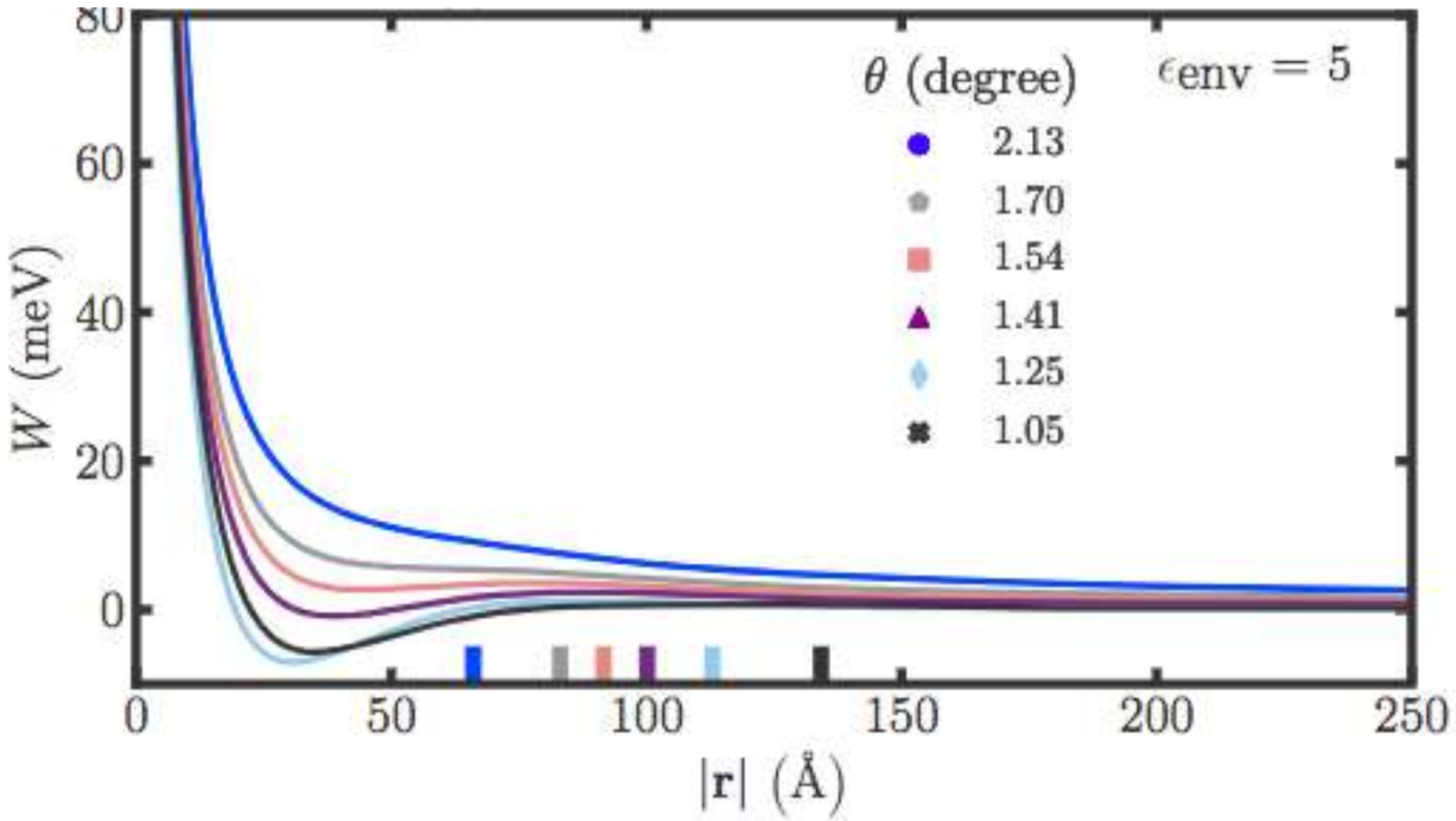
$$\Pi_0(\mathbf{q}) = \frac{4}{\Omega} \sum_{\mathbf{k}\in 1BZ} \sum_{cv} \frac{|\langle \psi_{v\mathbf{k}} | e^{-i\mathbf{q}\cdot\mathbf{r}} | \psi_{c\mathbf{k}+\mathbf{q}} \rangle|^2}{\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}+\mathbf{q}}}$$



Goodwin et al., Phys. Rev. B 100, 235424 (2019)

INTERNAL SCREENING

Attractive interactions



Goodwin et al., Phys. Rev. B 100, 235424 (2019)

POLARIZATION GLUE?

NEW MECHANISM FOR SUPERCONDUCTIVITY*

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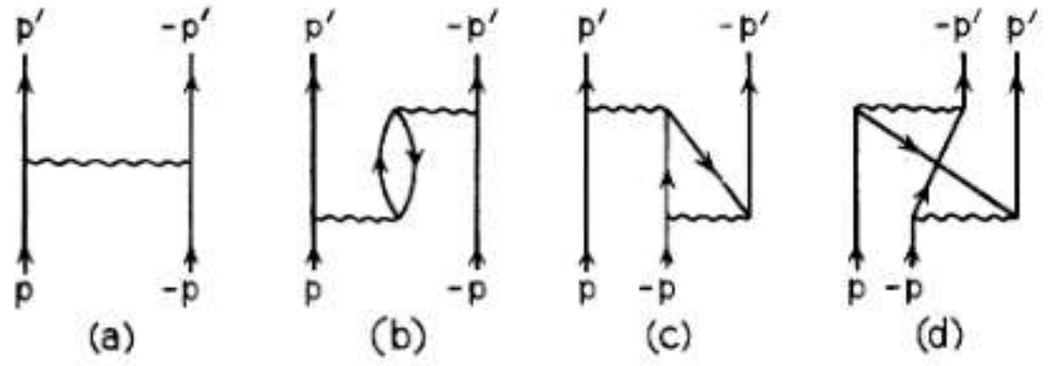
(Received 16 August 1965)

To understand what is involved, we first take an over-simplified view of the effect. It has long been known[1] that if a charge is placed in a metal, the screening is such that there remains a long-range oscillatory potential of the form $\cos(2k_F r+\varphi)/r^3$ (k_F is the Fermi momentum). This leads to a long-range interaction between charges. Formally, the source

It is plausible to suppose that, similarly, the effective interaction between the fermions themselves will have a long-range oscillatory part. By taking advantage of the attractive regions, Cooper pairs can form thus giving rise to superconductivity.



Kohn, Luttinger, Phys. Rev. Lett. 15, 524 (1965)

ELECTRONIC PROPERTIES OF TWISTED BILAYER GRAPHENE

Summary:

- importance of long-ranged interactions revealed in normal state
- new opportunities to probe electron correlations in two dimensions
- twisted bilayer graphene might be very different from the cuprates after all
- internal screening might provide superconducting glue

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THE ROYAL SOCIETY