ICTP Summer School, Sep 22. 2023, Bukhara, Uzbekistan

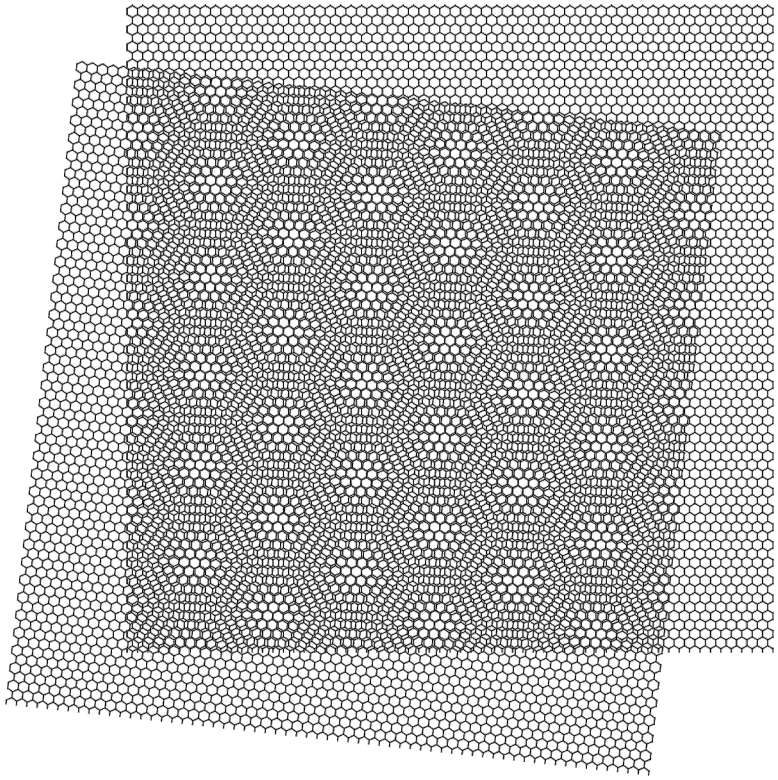
Exploring Moiré 2D Materials and Topological Quasicrystals

Mikito Koshino (Osaka Univ.)

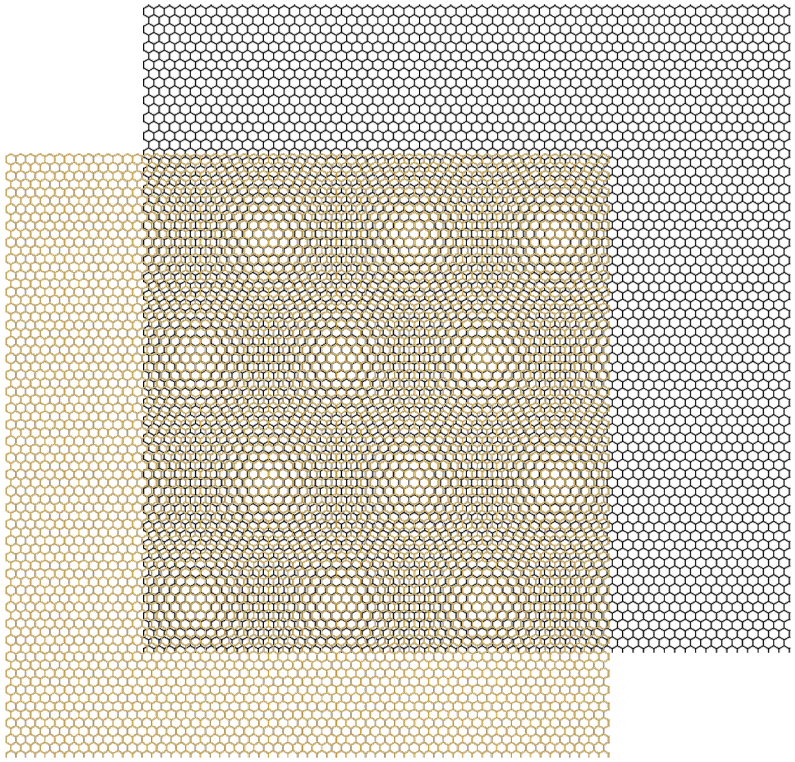
Grant-in-Aid for Transformative Research Areas(A)
Science of 2.5 Dimensional Materials
Paradigm Shift of Materials Science Toward Future Social Innovation
2.5D Materials

Moiré 2D materials

Homo-bilayer
(moiré pattern from rotation)

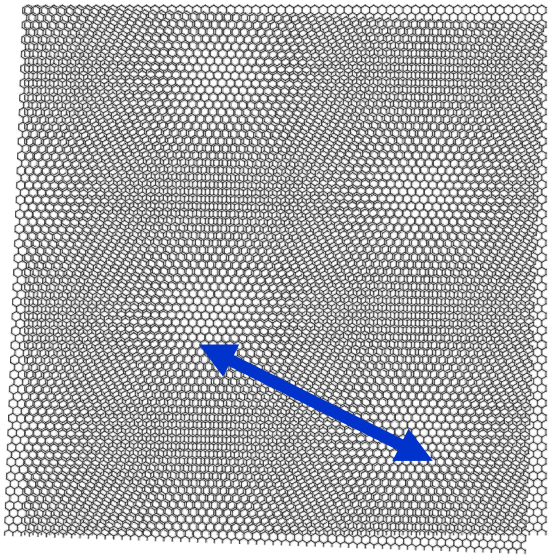


Hetero-bilayer
(moiré pattern from lattice mismatch)



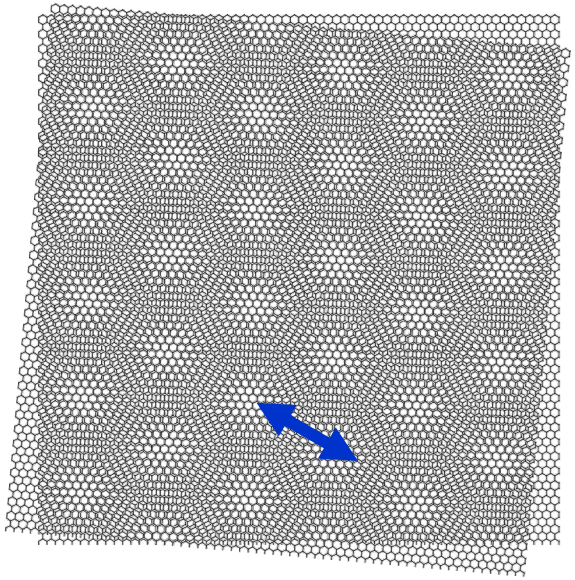
Twisted bilayer graphene (TBG)

$\theta = 2^\circ$



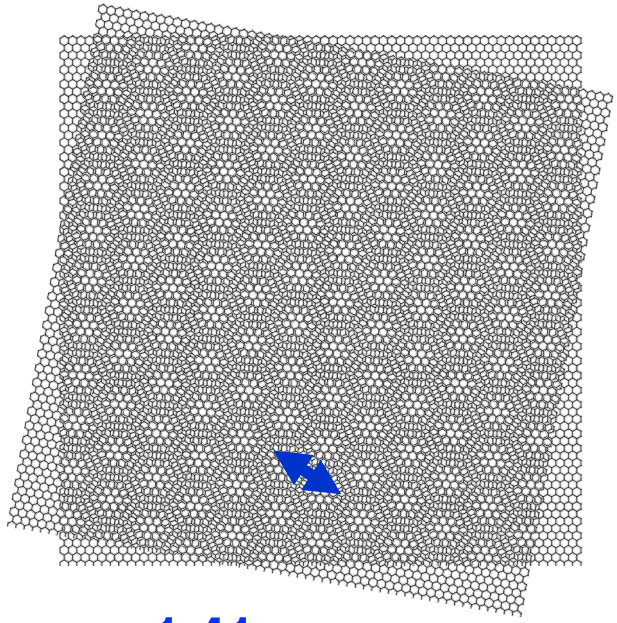
L = 7.04nm

$\theta = 5^\circ$



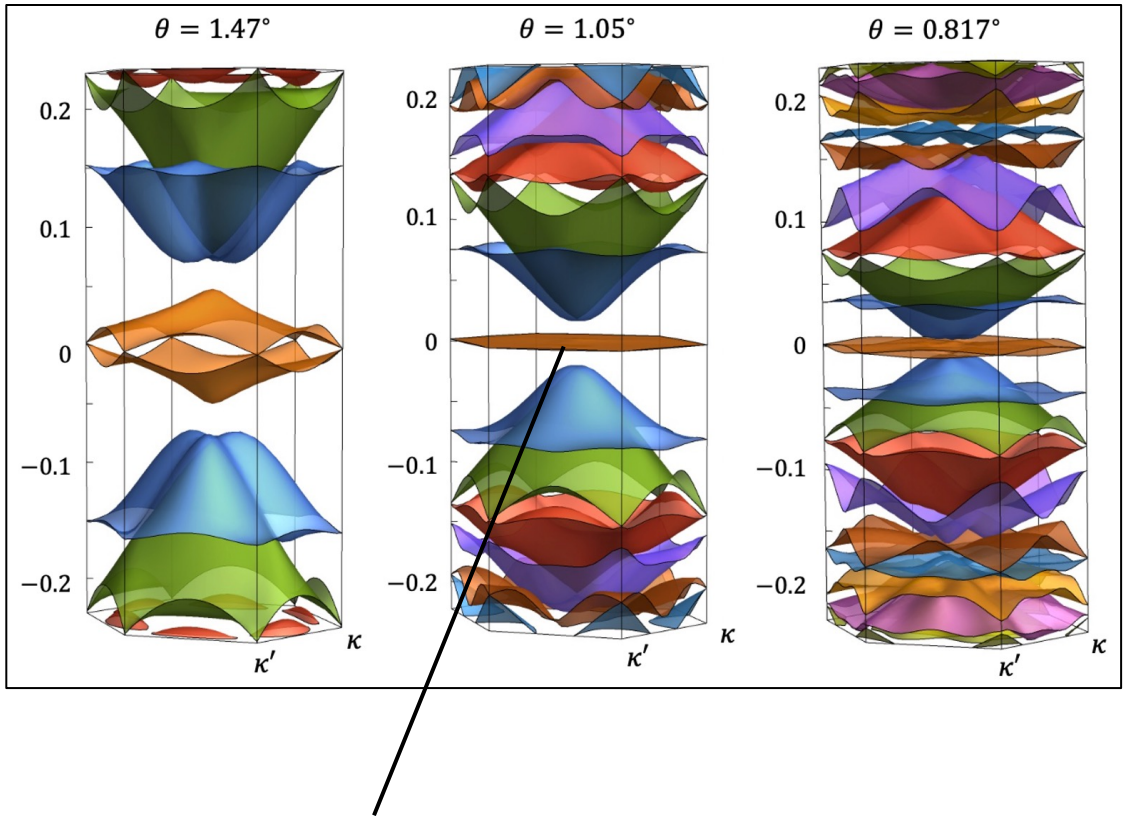
2.82nm

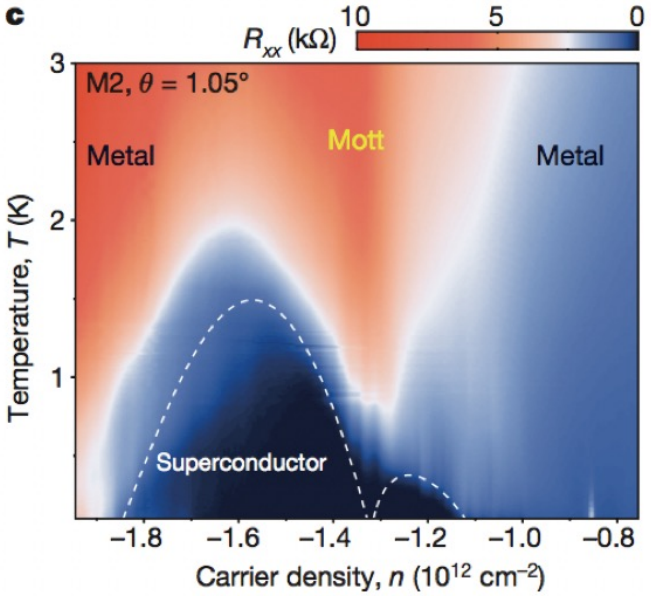
$\theta = 10^\circ$



1.41nm

Flat band and superconductivity





Flat bands at a magic angle

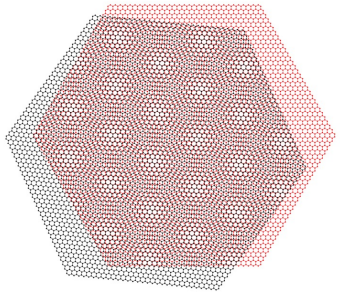
R. Bistritzer and A. MacDonald, PNAS 108, 12233 (2011).

Correlated Insulating states and superconductivity at magic angle

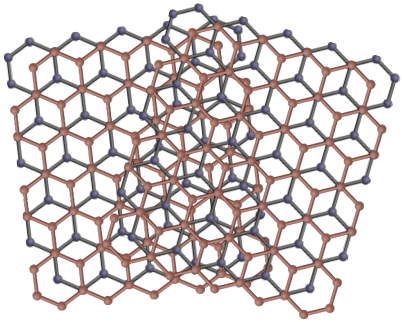
Y. Cao et al, Nature 556, 43 (2018)
Y. Cao et al, Nature 556, 80 (2018) →
M. Yankowitz et al., Science 363, 1059 (2019).

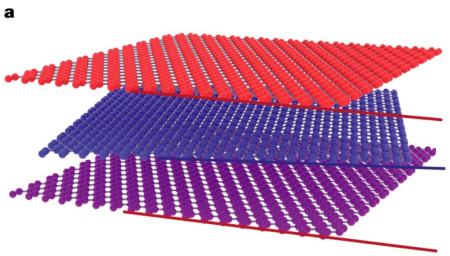
Family of moiré 2D materials

Twisted bilayer graphene



Twisted multilayer graphenes

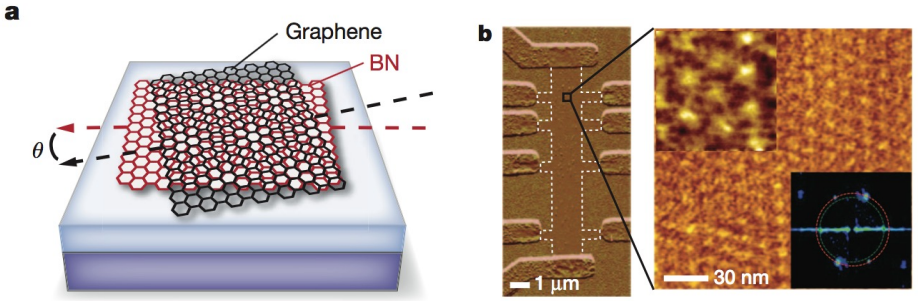




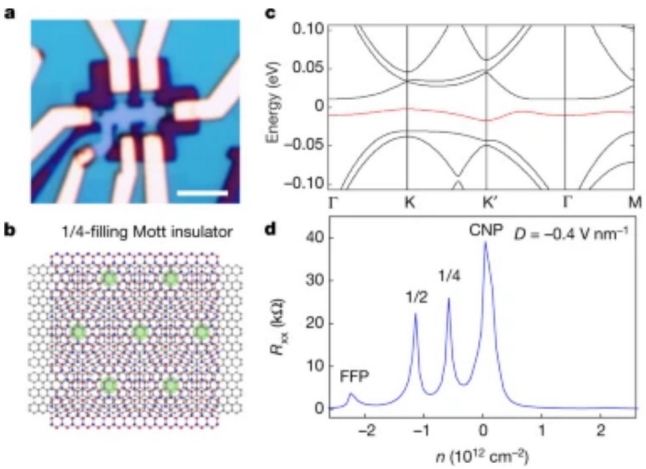
Park et al, Nature 590, 249 (2021)

Graphene-hBN

Dean, et al, Nature 497, 598 (2013)

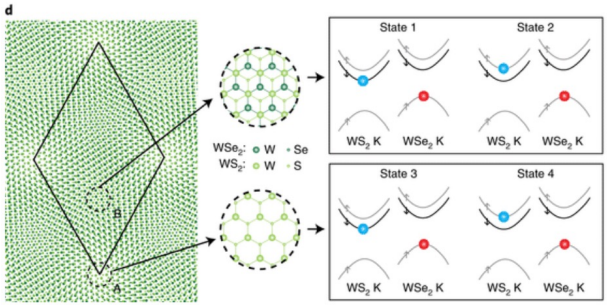


ABC-trilayer graphene-hBN



Chen et al Nature 572, 215 (2019)

TMDC-TMDC

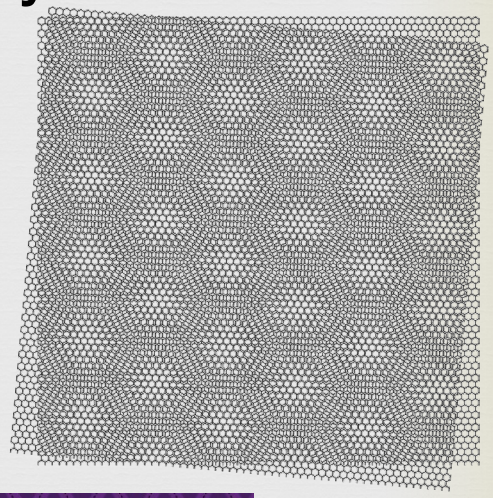


C. Jin et al,
Nat. Phys. 15, 1140 (2019)

Outline: Physics of moiré materials & beyond

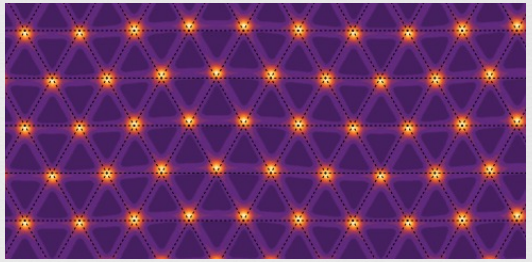
Twisted bilayer graphene

-- Moiré electron bands and continuum model



Moiré phonons

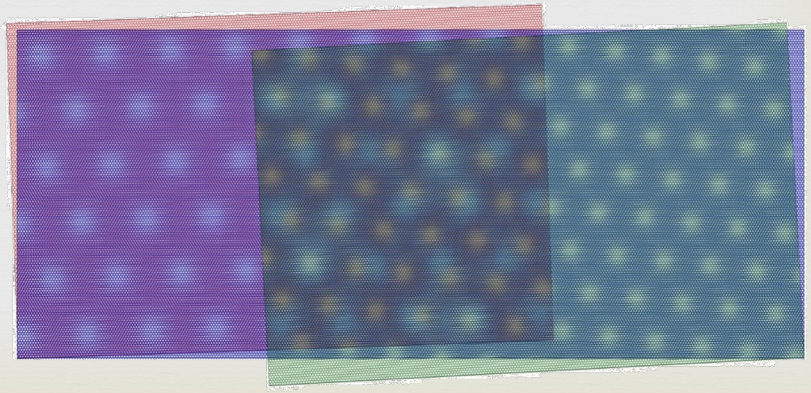
-- Vibration of “moiré atoms”

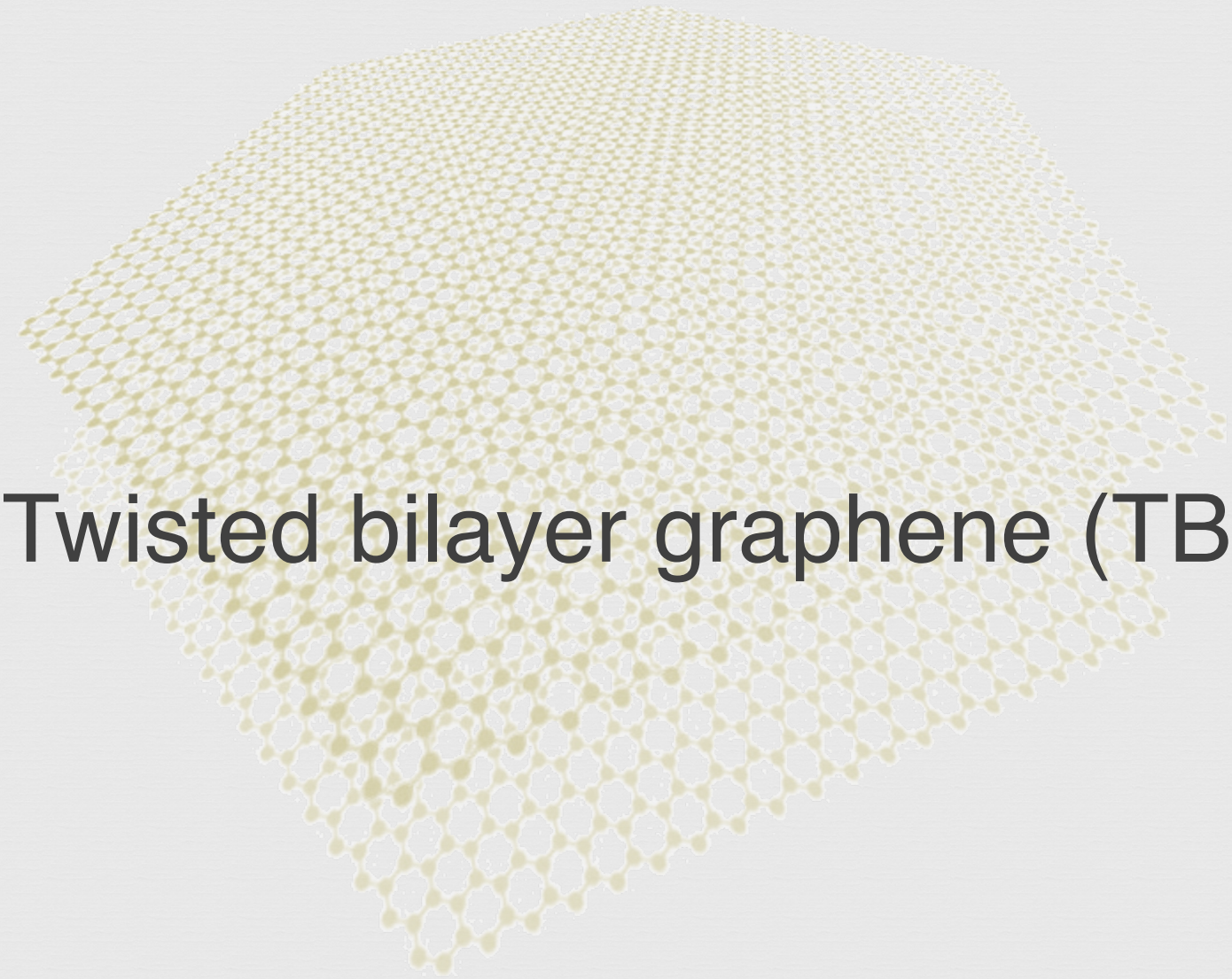


Moiré trilayer systems

-- moiré-of-moiré quasicrystal

-- topological gap labeling



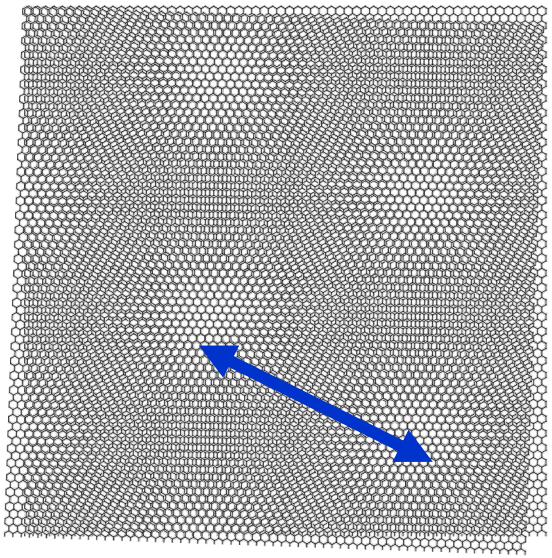


Twisted bilayer graphene (TBG)

Moiré period

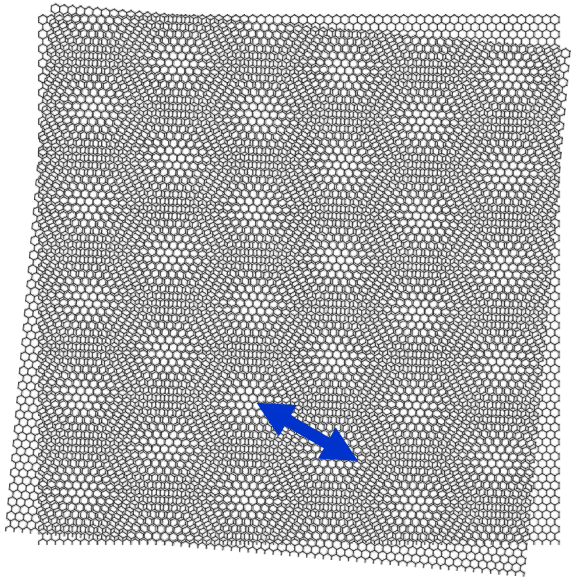
$$L = \frac{a}{2\sin\frac{\theta}{2}}$$

$\theta = 2^\circ$



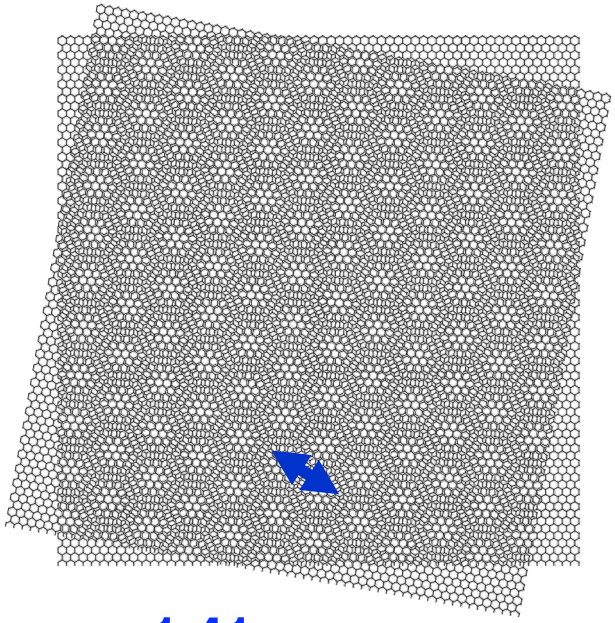
L = 7.04nm

$\theta = 5^\circ$



2.82nm

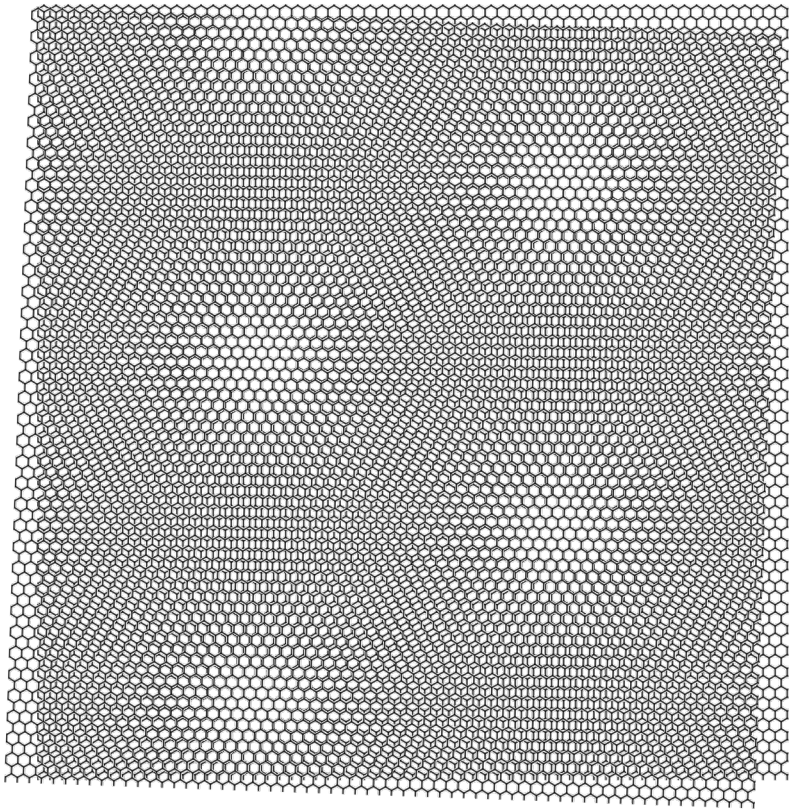
$\theta = 10^\circ$



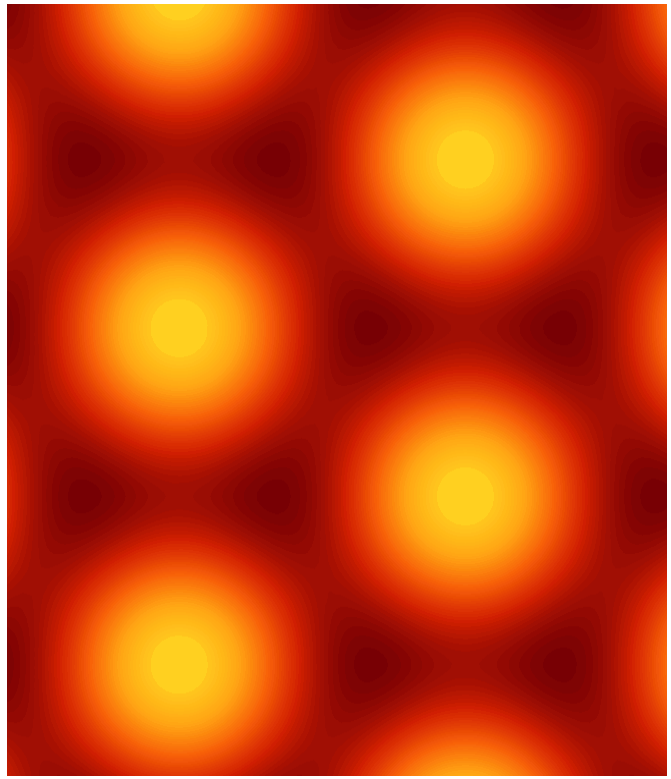
1.41nm

Continuum model

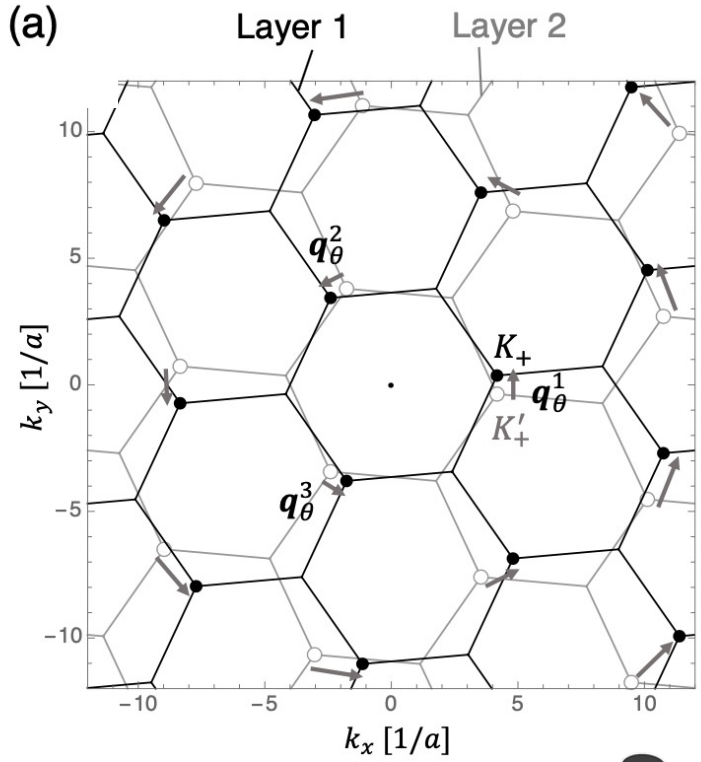
Huge number of atoms
(10,000 at $\theta = 1^\circ$)

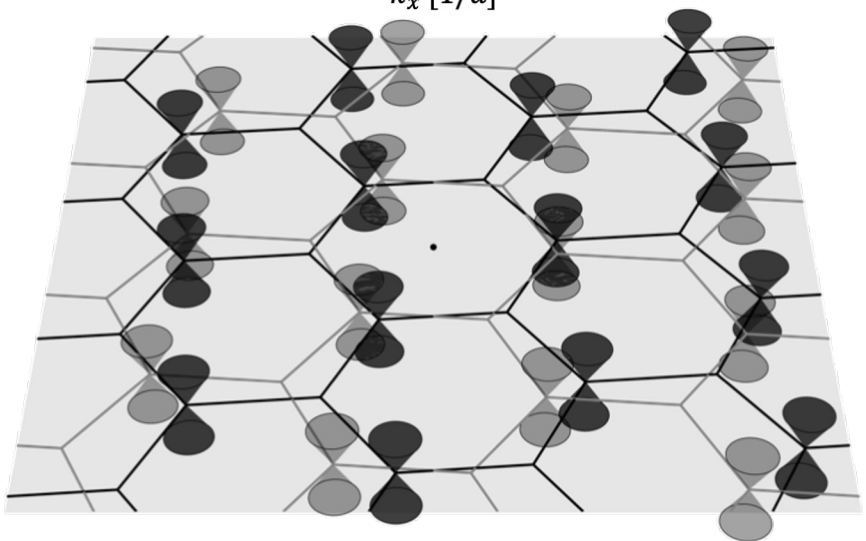


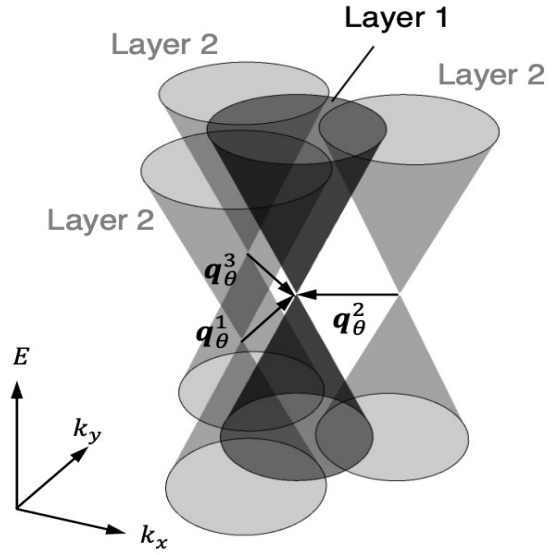
Coarse-graining
to extract the long-wave components

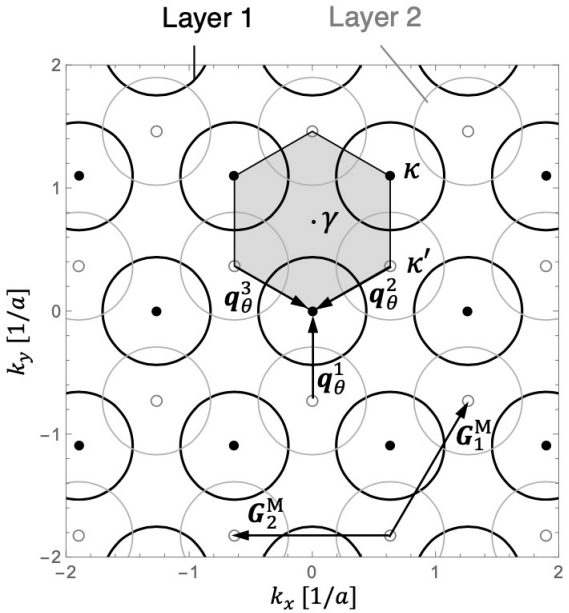


Continuum model (k-space picture)









Continuum Hamiltonian

Lopes dos Santos et al, PRL 99, 256802 (2007)
Bistritzer and MacDonald, PNAS 108, 12233 (2011)
Kindermann and First, PRB 83, 045425 (2011)
Moon and Koshino, PRB 87, 205404 (2013)

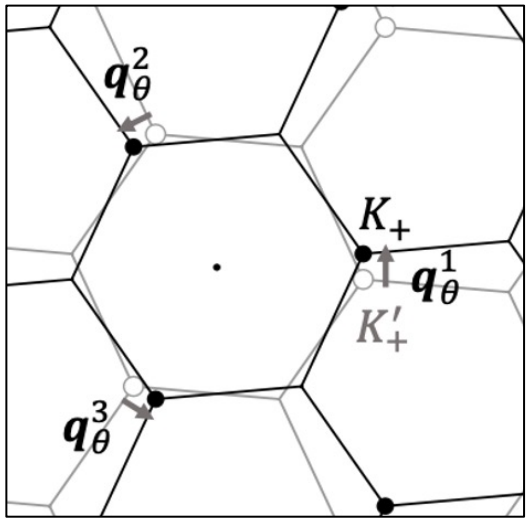
$$H_{\text{eff}} = \begin{pmatrix} H_0 & U^\dagger \\ U & H_0 \end{pmatrix}$$

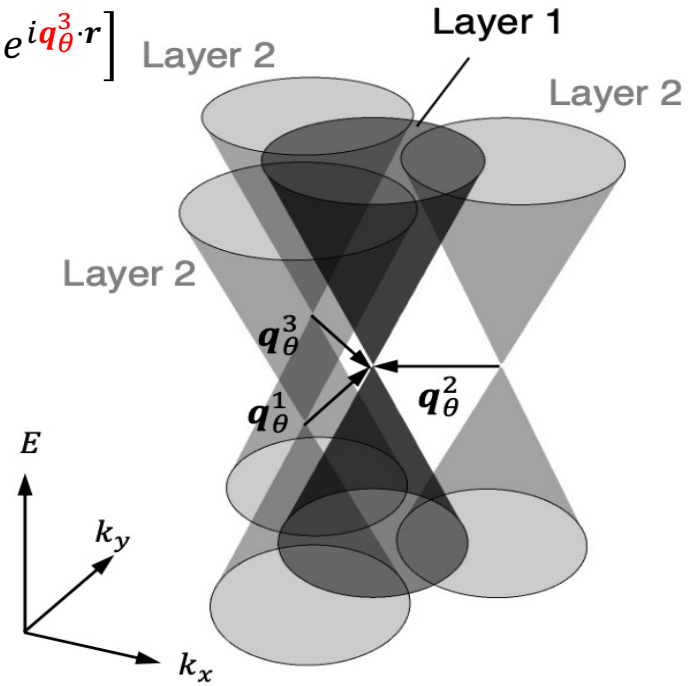
graphene's Dirac Hamiltonian

$$H_0 = v\boldsymbol{\sigma}\cdot\boldsymbol{p}$$

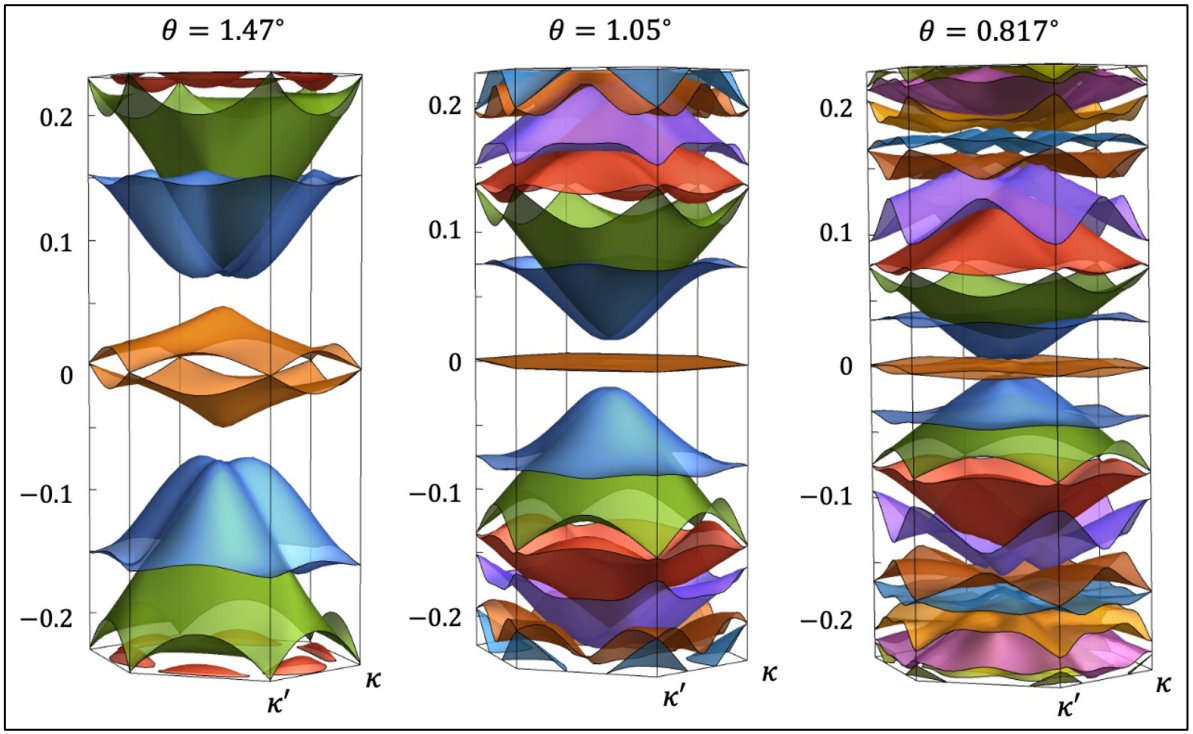
Moiré interlayer coupling:

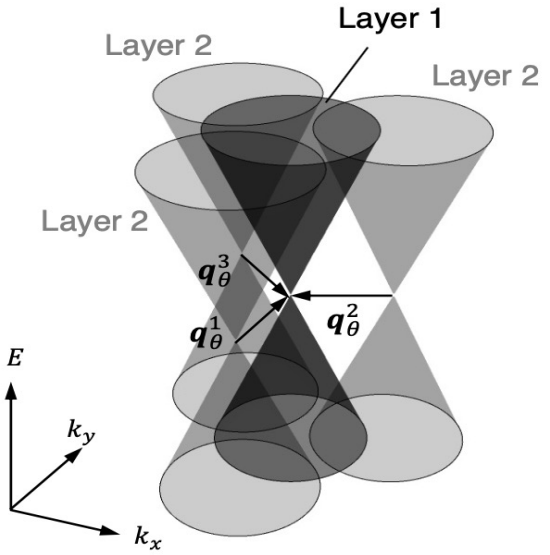
$$\begin{pmatrix} U_{AA} & U_{AB} \\ U_{BA} & U_{BB} \end{pmatrix} = u_0 \left[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} e^{i\boldsymbol{q}_\theta^1\cdot\boldsymbol{r}} + \begin{pmatrix} 1 & \omega^* \\ \omega & 1 \end{pmatrix} e^{i\boldsymbol{q}_\theta^2\cdot\boldsymbol{r}} + \begin{pmatrix} 1 & \omega \\ \omega^* & 1 \end{pmatrix} e^{i\boldsymbol{q}_\theta^3\cdot\boldsymbol{r}} \right]$$

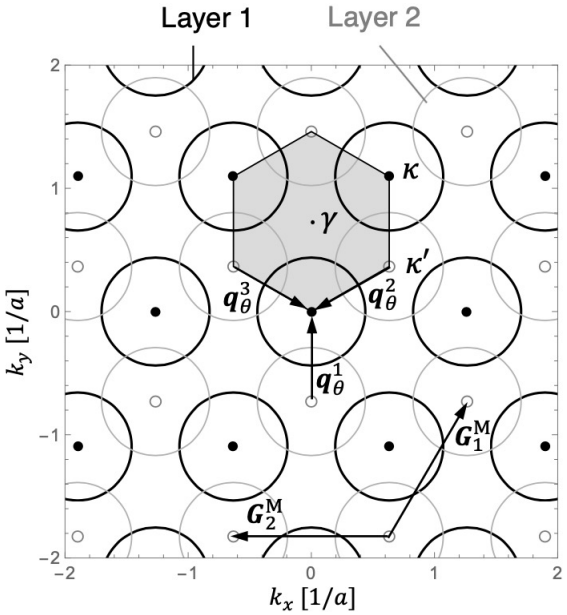




Band structure of TBG

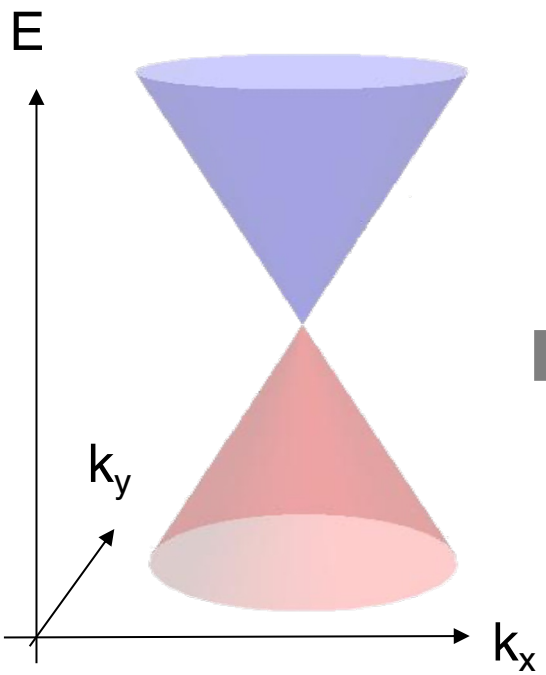


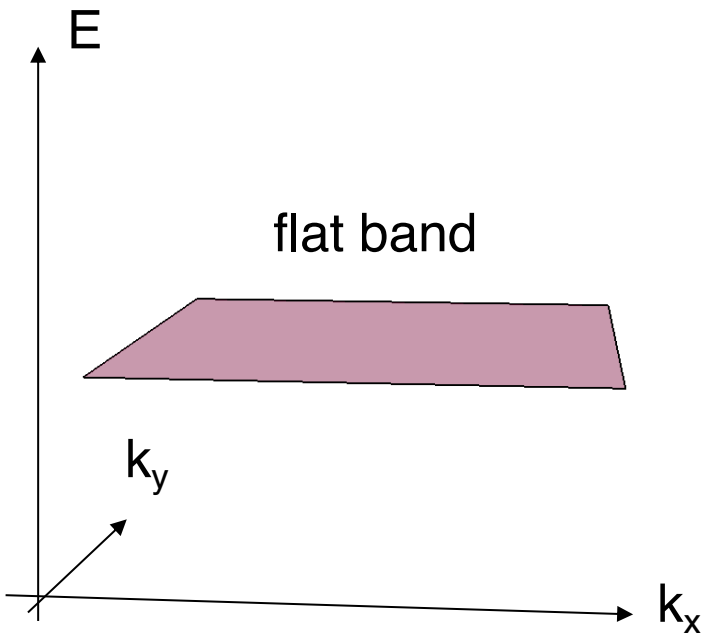




Flat band physics

Total energy of electrons = **kinetic energy** + **potential energy**
(band energy) (electron-electron interaction)





No kinetic energy

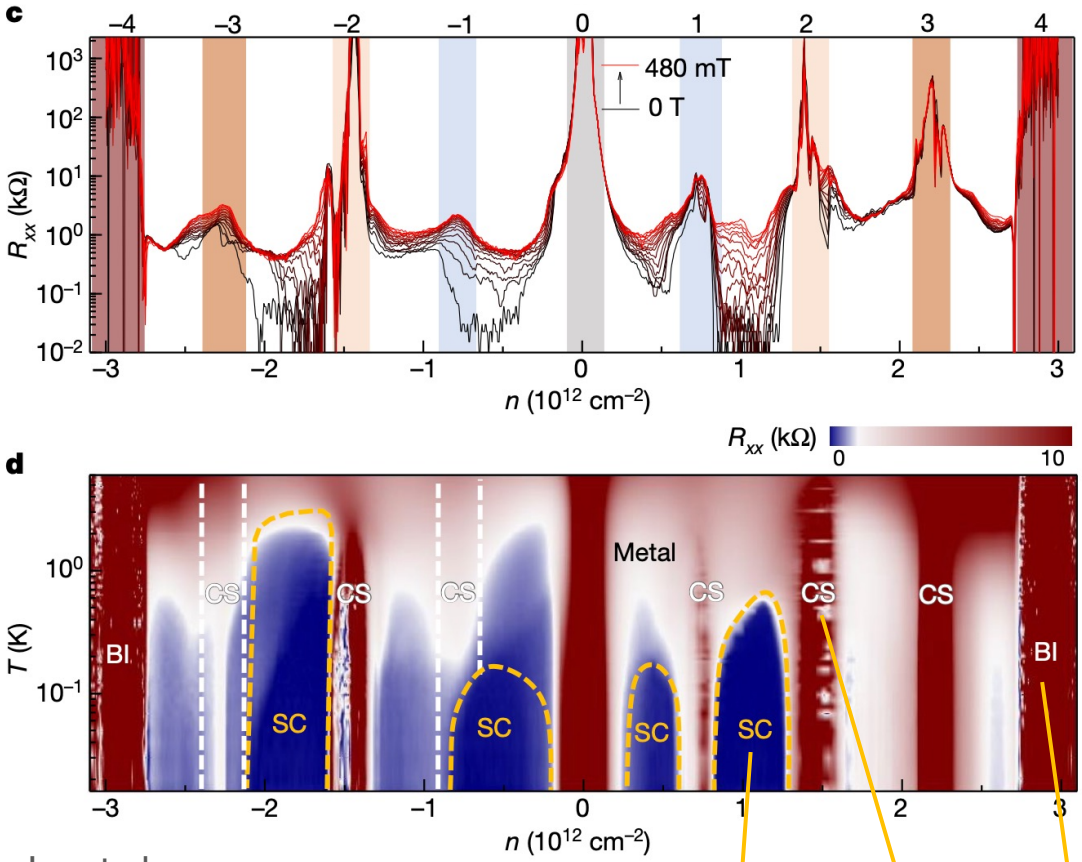
→ physics is governed by
electron-electron interaction!

Correlated insulating states & superconductivity

θ = 1.10°

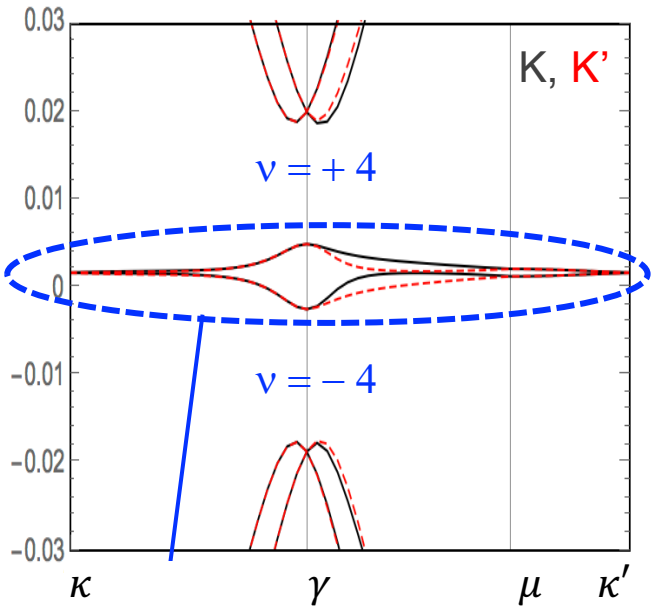
Band filling
(number of the occupied minibands)

ν



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

θ = 1.05°

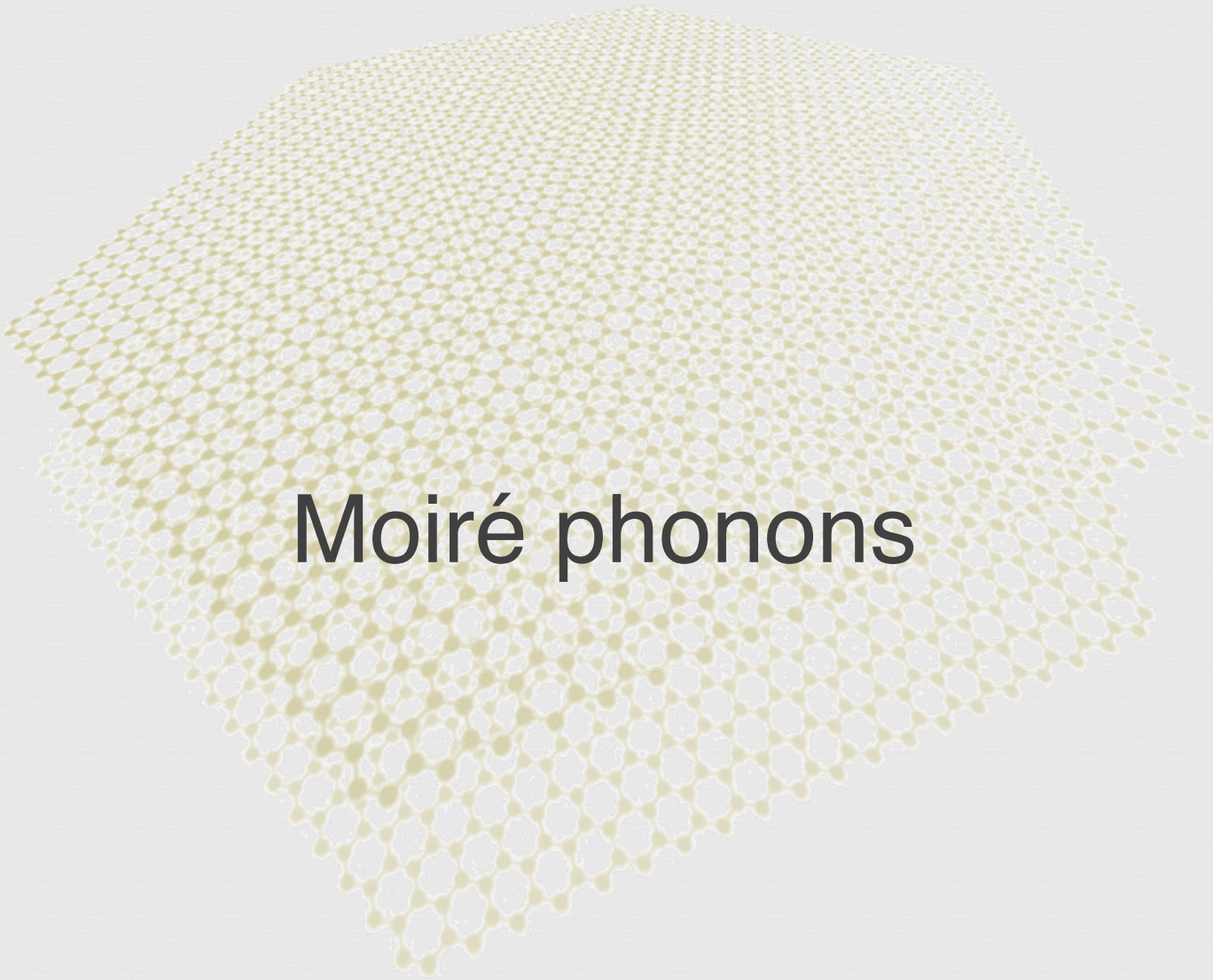


8 minibands
(including spin and valleys)

Band insulator

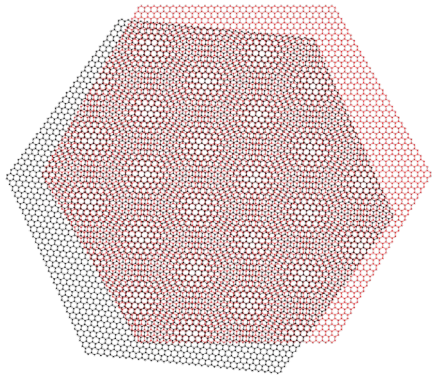
Superconducting

Correlated insulator

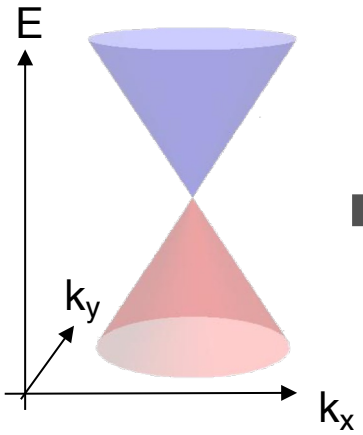


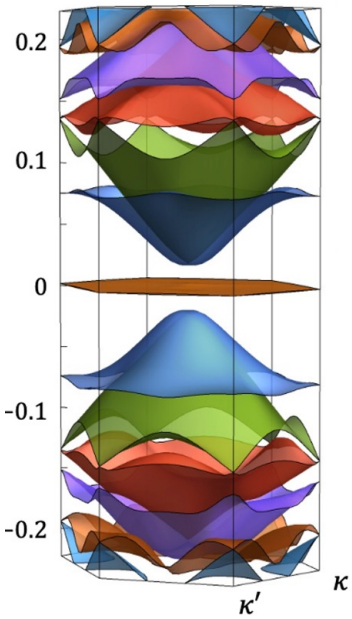
Moiré phonons

Moiré phonons?

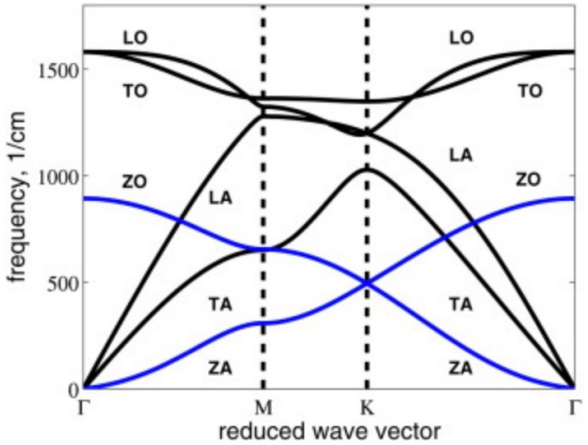


Electronic band





Phonon band

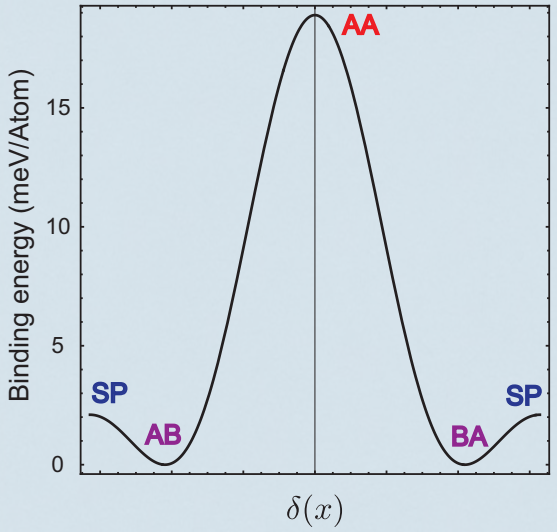


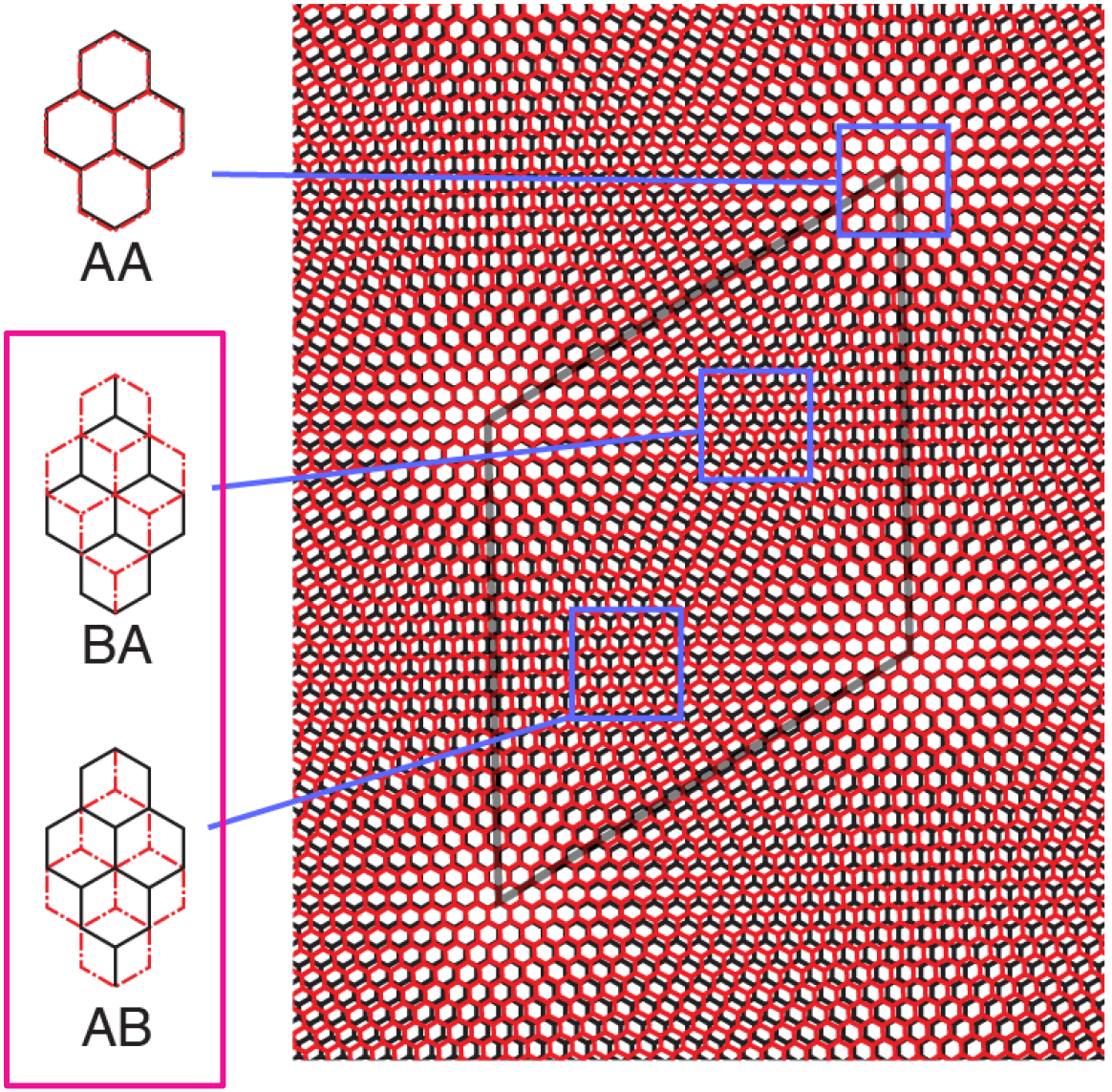
?

Local stacking structure in TBG

AA: highest energy

AB / BA: lowest energy



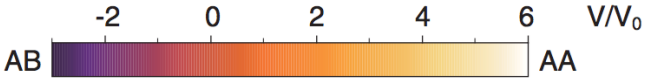


Lattice relaxation of TBG

Nam and Koshino,
Phys. Rev. B 96, 075311 (2017)

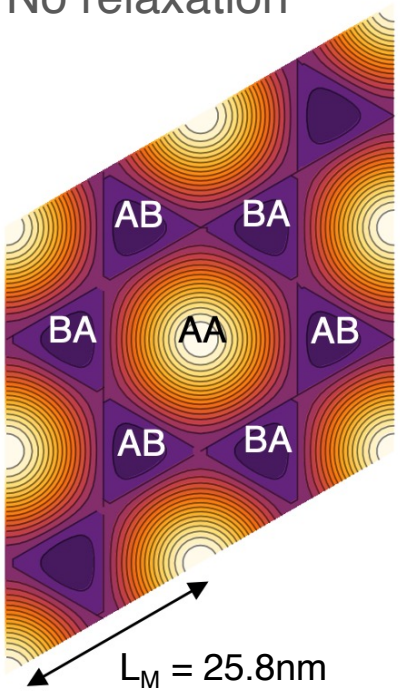
N. N. T. Nam
(Tohoku)

Local binding energy

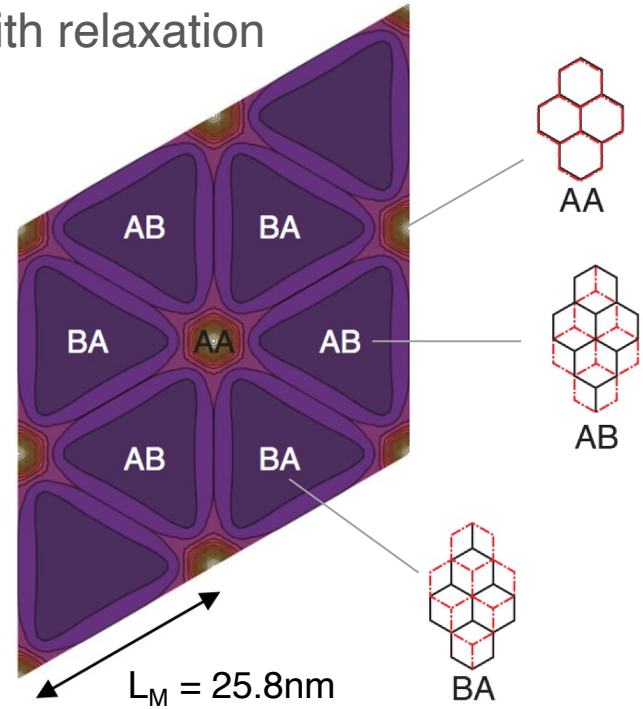


ex.) $\theta = 0.547°$

No relaxation



With relaxation



See also:

K. Uchida, S. Furuya, J.-I. Iwata, and A. Oshiyama, Phys. Rev. B 90, 155451 (2014).
M. van Wijk, A. Schuring, M. Katsnelson, and A. Fasolino, 2D Mater. 2, 034010 (2015).
S. Dai, Y. Xiang, and D. J. Srolovitz, Nano Lett. 16, 5923 (2016).
S. K. Jain, V. Jurivci'c, and G. T. Barkema, 2D Mater. 4, 015018 (2016).

Theoretical method ––– continuum approach

N. N. T. Nam
(Tohoku)

Nam and Koshino,
Phys. Rev. B 96, 075311 (2017)

Elastic energy

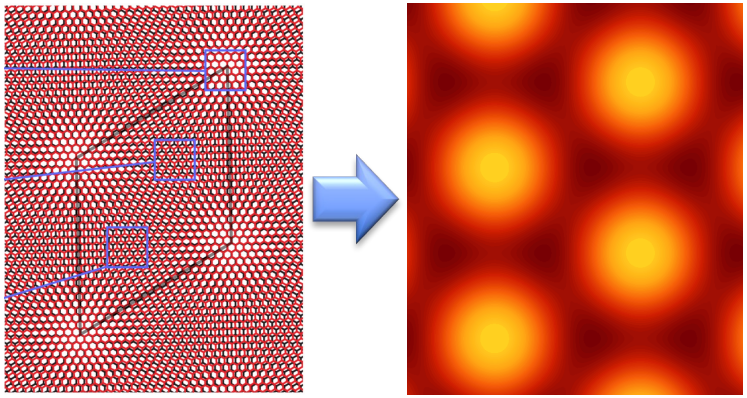
$$U_E = \sum_{l=1}^{2} \int \frac{1}{2} \left\{ (\lambda+\mu)(u_{xx}^{(l)} + u_{yy}^{(l)})^2 + \mu \left[(u_{xx}^{(l)} - u_{yy}^{(l)})^2 + 4(u_{xy}^{(l)})^2 \right] \right\} d^2\mathbf{r}$$

$u_{ij}^{(l)} = (\partial_i u_j^{(l)} + \partial_j u_i^{(l)})/2$: strain tensor,
μ and λ : Lamé factors.

Binding energy

$$U_B = \int V[\delta(\mathbf{r})] \mathrm{d}^2\mathbf{r}.$$

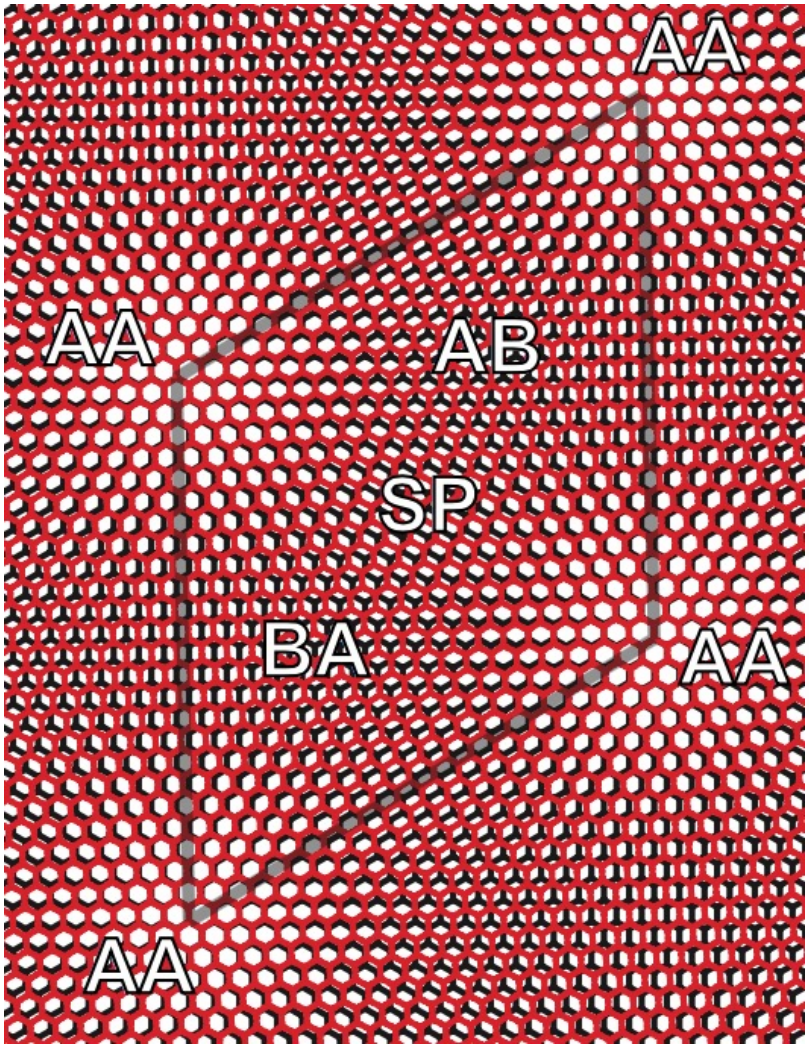
$$V[\delta(\mathbf{r})] = \sum_{j=1}^{3} 2V_0 \cos[\mathbf{G}_j^{\mathrm{M}} \cdot \mathbf{r} + \mathbf{a}_j^*(\mathbf{u}^{(2)} - \mathbf{u}^{(1)})]$$



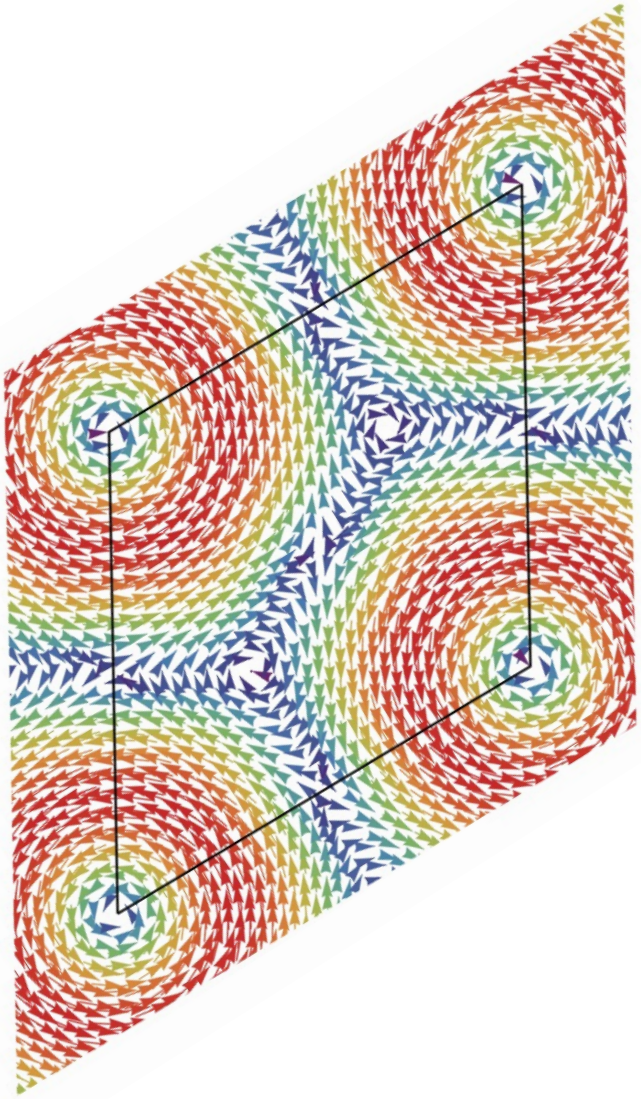
Minimize the total energy
(Numerically solving Euler-Lagrange equation)

Lattice distortion in atomic level

Original structure (No distortion)

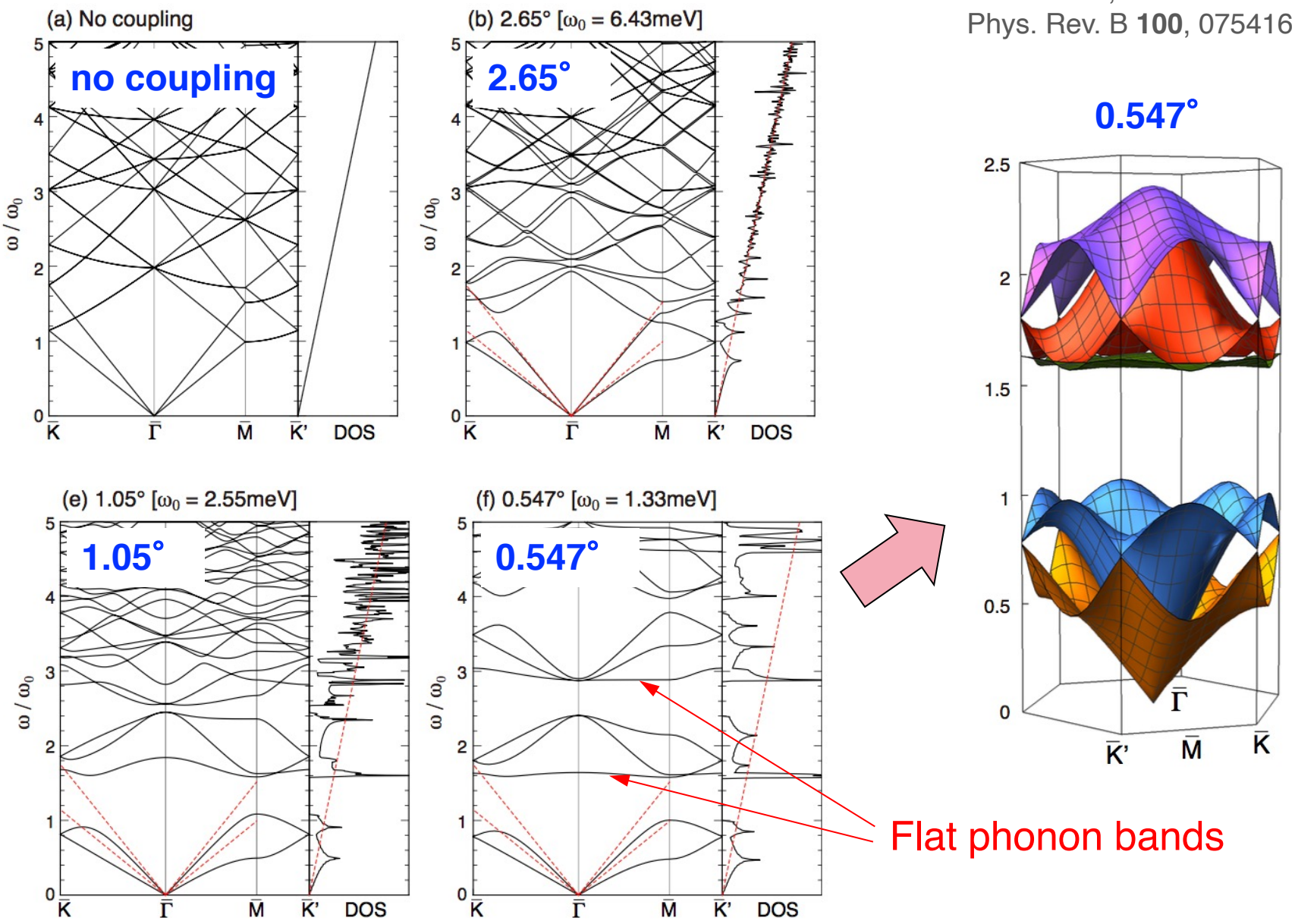


Displacement vector (layer 2)



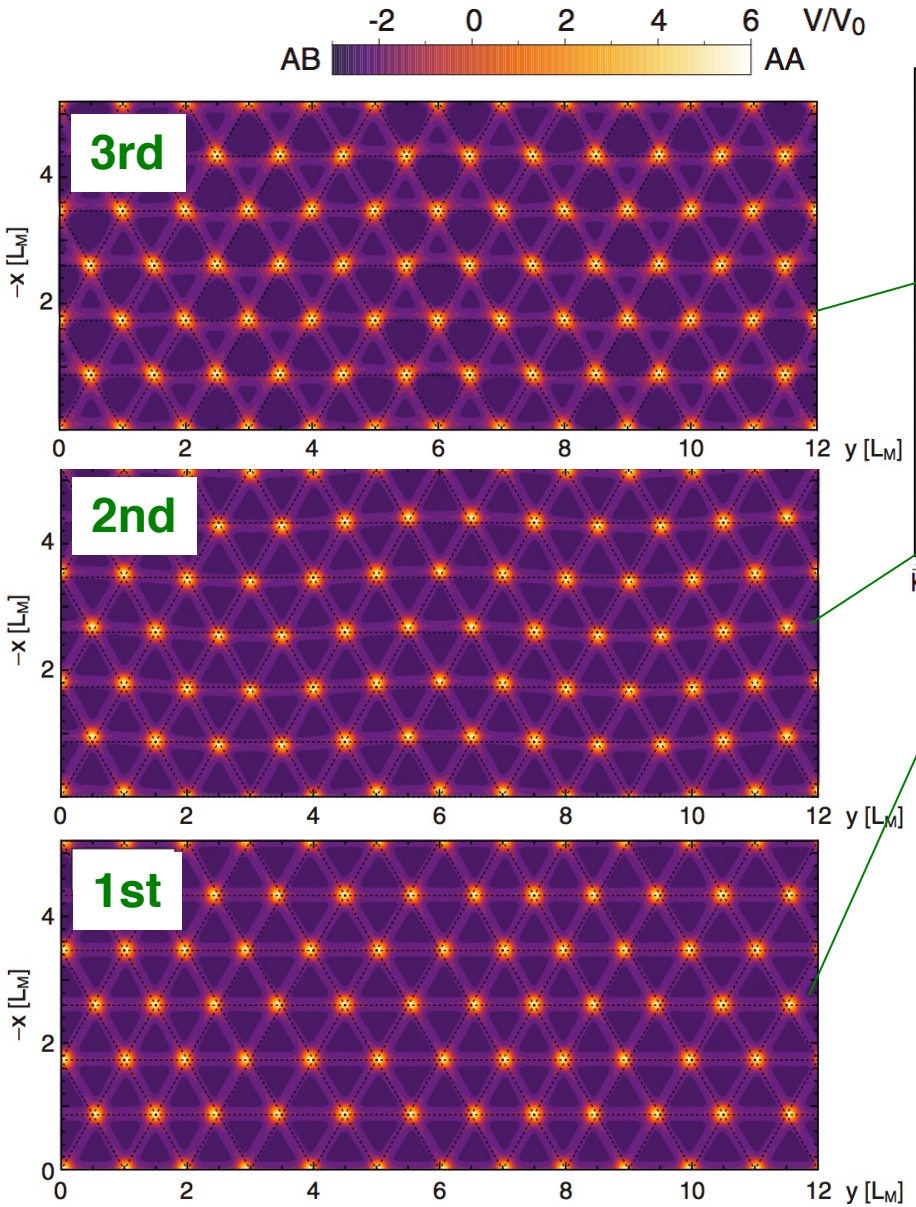
Moiré phonons in TBG

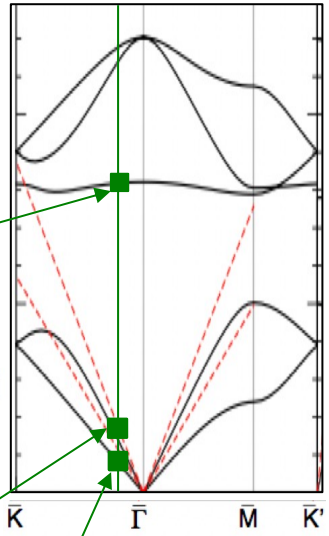
M. Koshino, and Y-.W. Son,
Phys. Rev. B **100**, 075416 (2019)

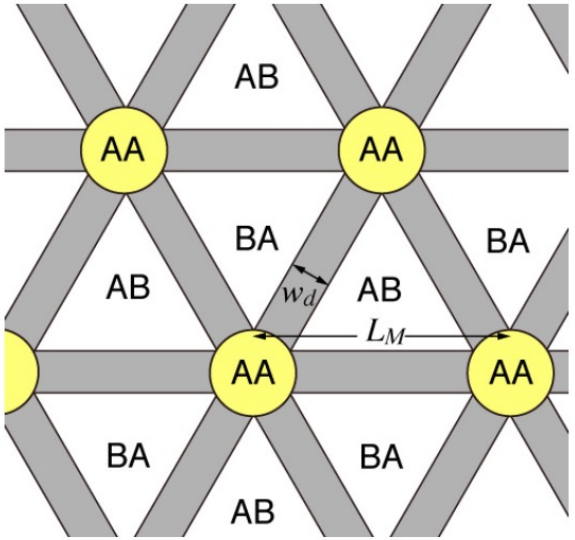


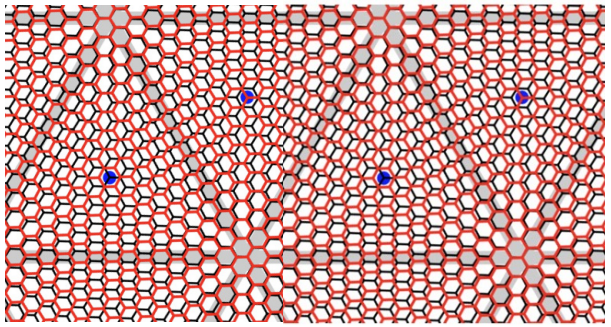
Moiré phonon wavefunctions

M. Koshino, and Y-.W. Son,
Phys. Rev. B **100**, 075416 (2019)
M. Koshino and NNT Nam,
Phys. Rev. B 101, 195425 (2020)









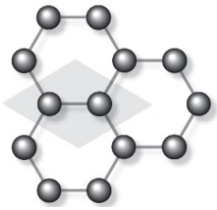
Vibration of ”big atoms”

Moiré phonons in G/hBN

Krishna and Koshino,
Phys. Rev. B 107, 115301 (2023)

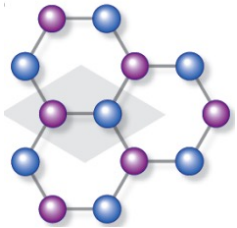
Lukas Krisna
(Osaka)

Graphene



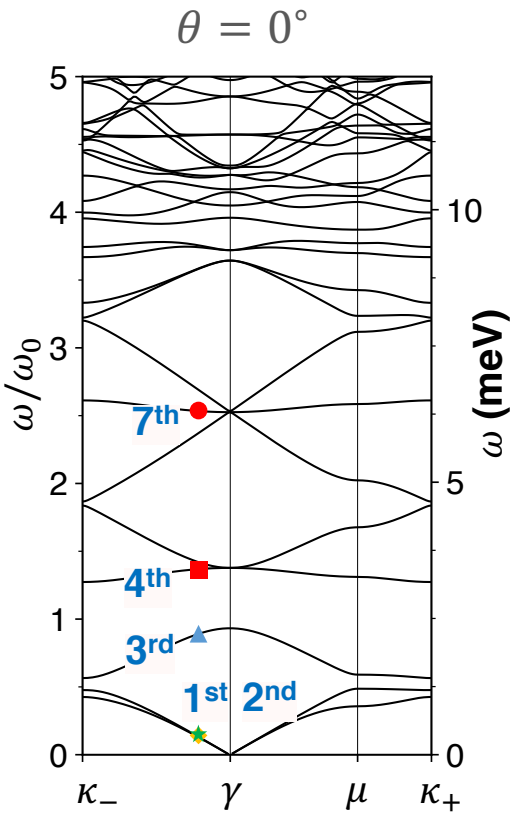
C

h-BN

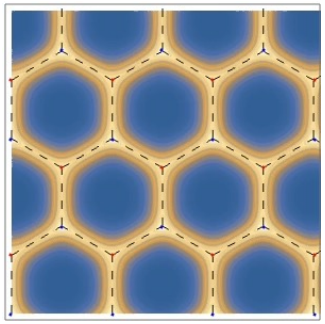


B N

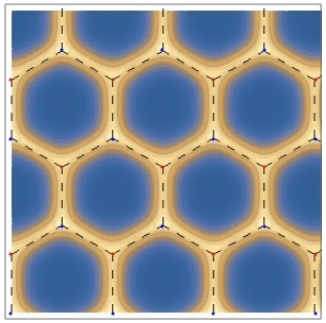
1.8 % lattice constant mismatch



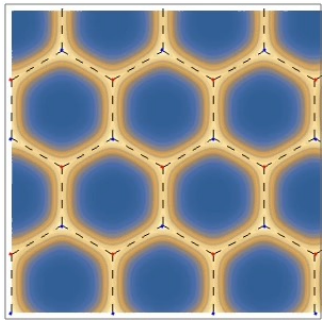
1st



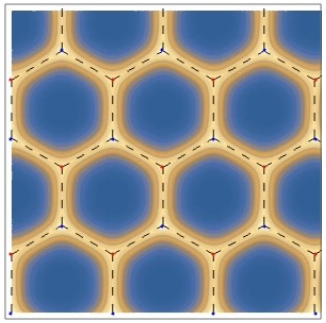
2nd



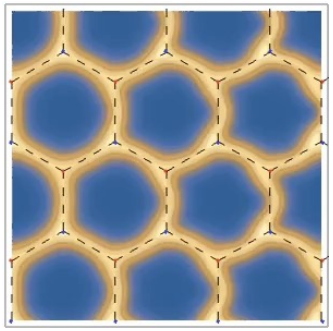
3rd



4th



7th

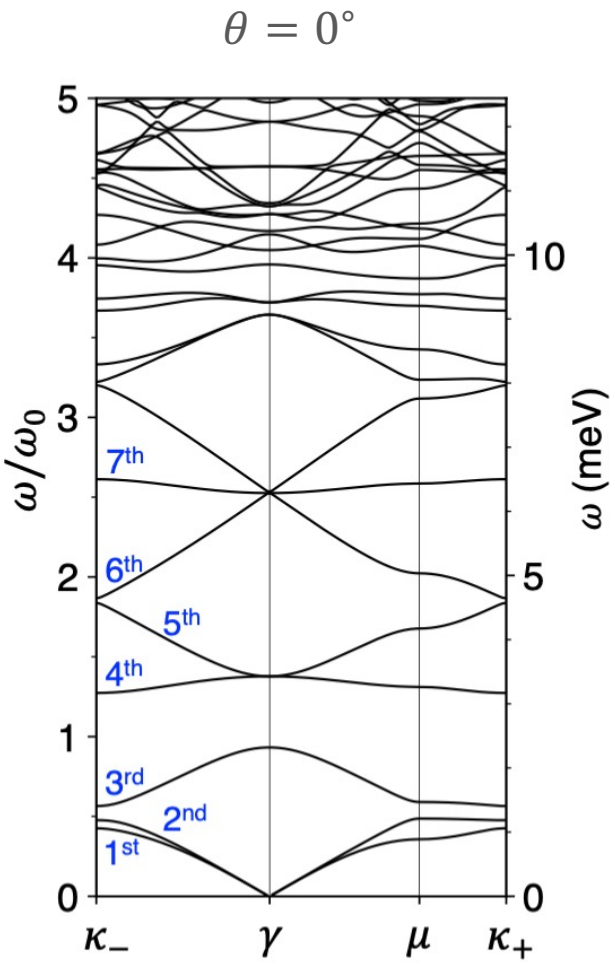


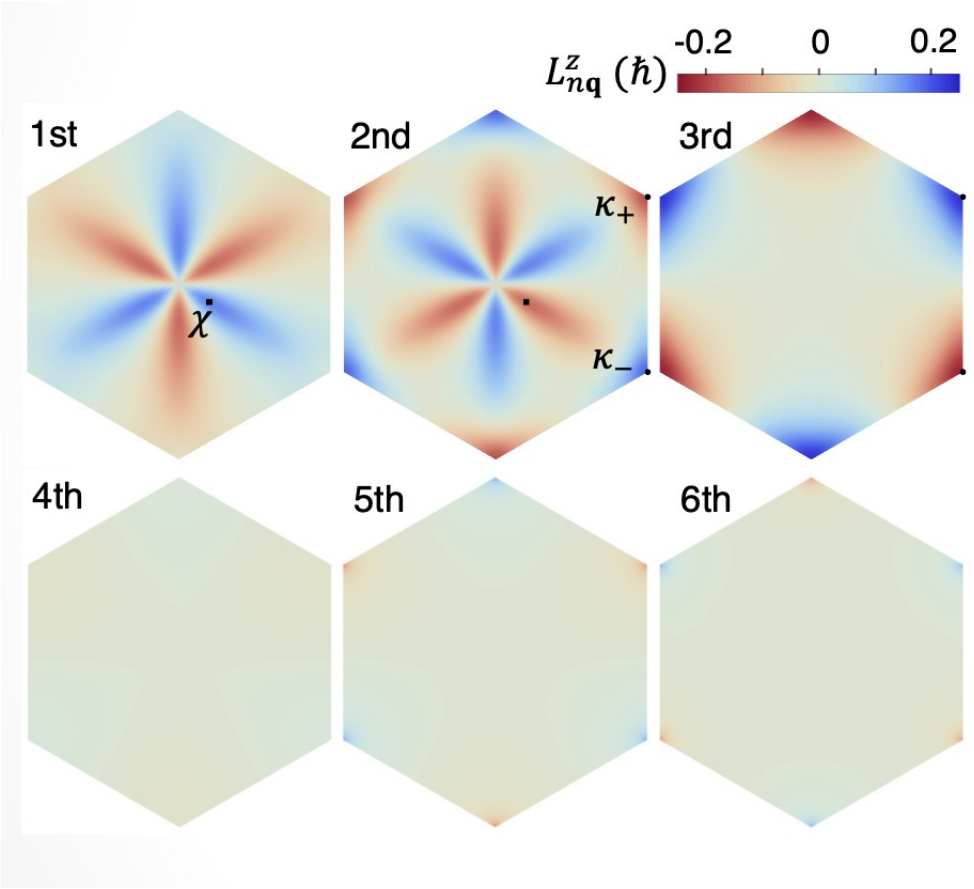
“Chiral phonons” in G/hBN

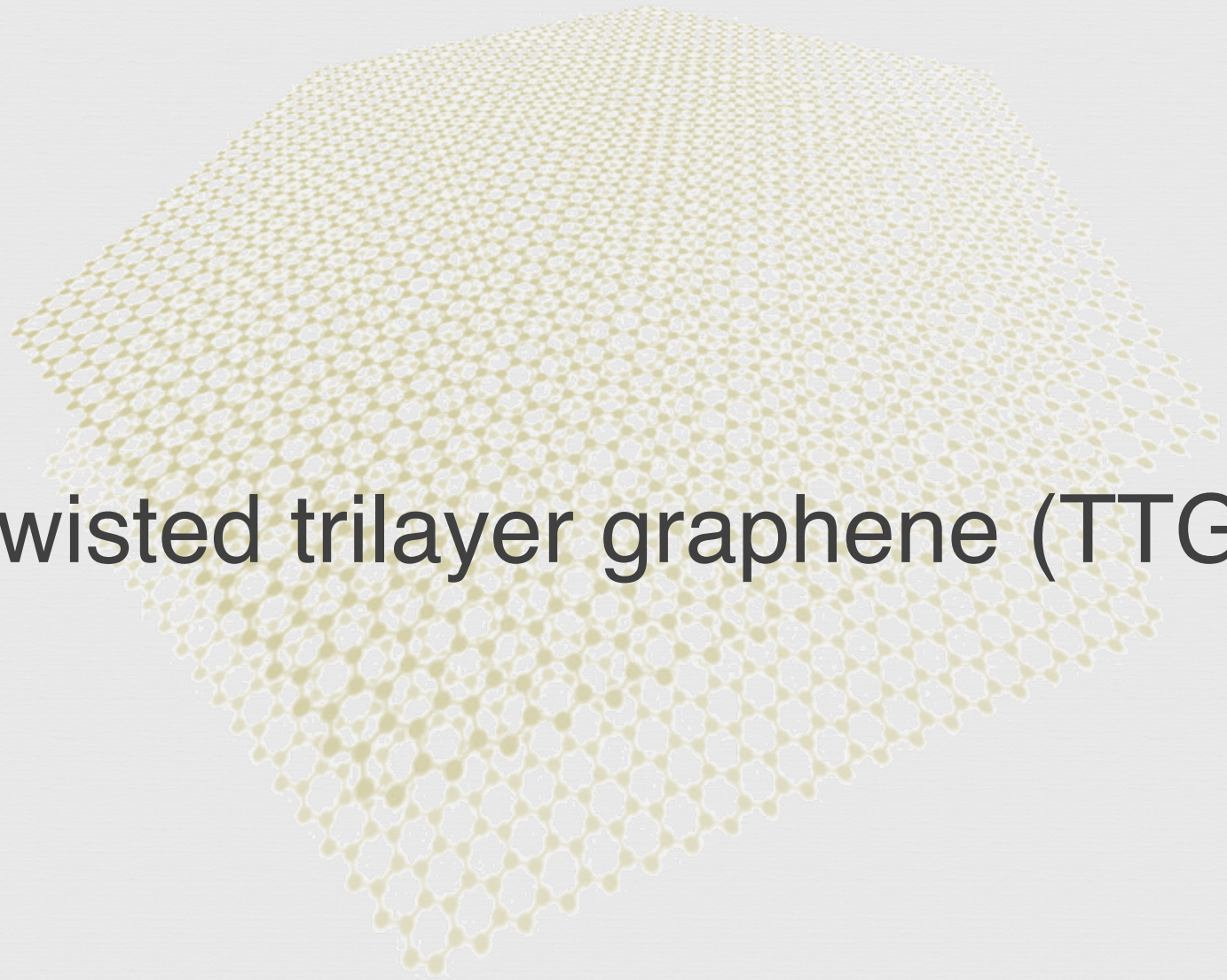
Krishna and Koshino,
Phys. Rev. B 107, 115301 (2023)

G/hBN: inversion symm. broken

Angular momentum in phonons



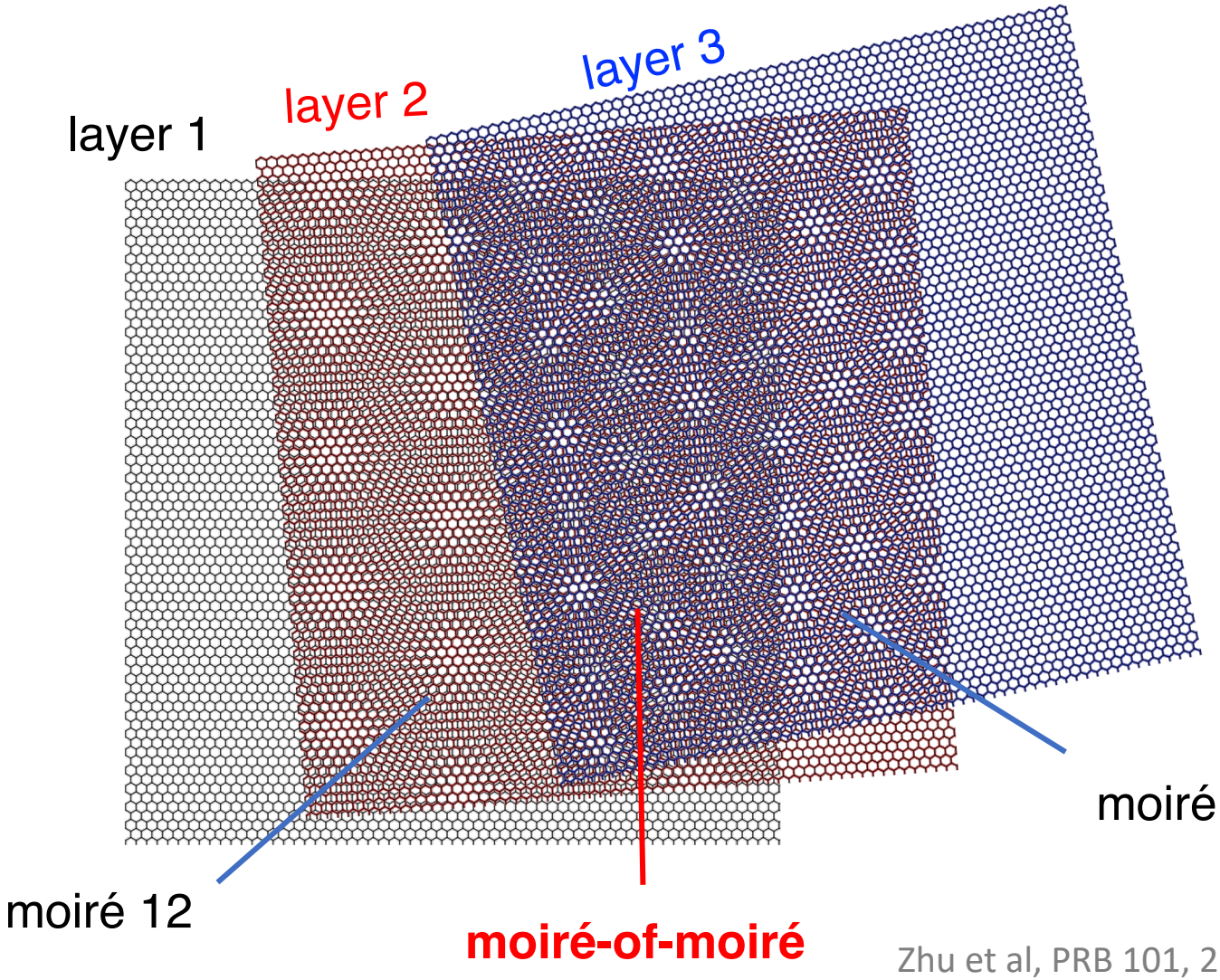




Twisted trilayer graphene (TTG)

Twisted trilayer graphene (TTG)

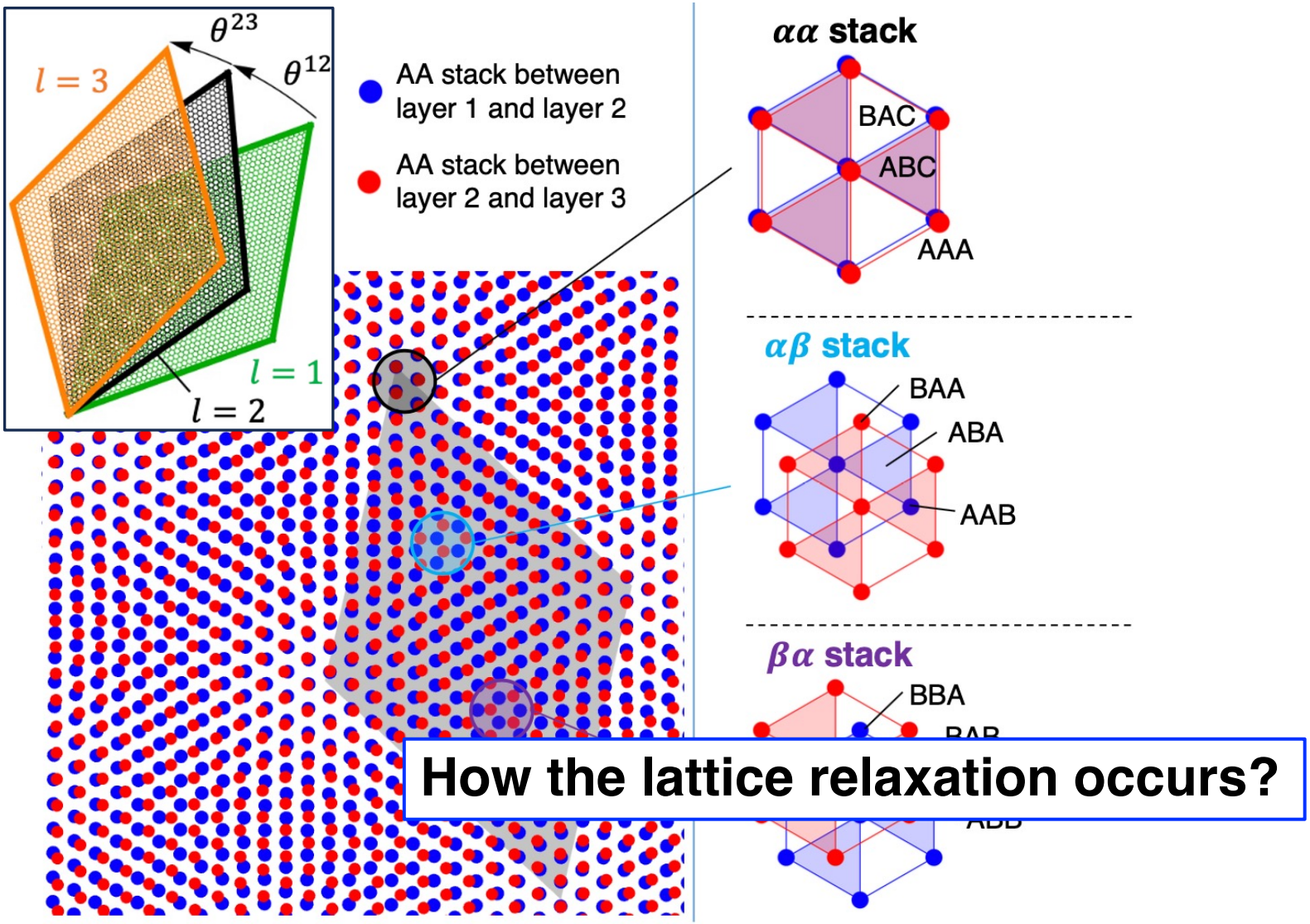
Naoto Nakatsuji
(Osaka)



Zhu et al, PRB 101, 224107 (2020)
Zhang et al. PRL 127, 166802 (2021)
…

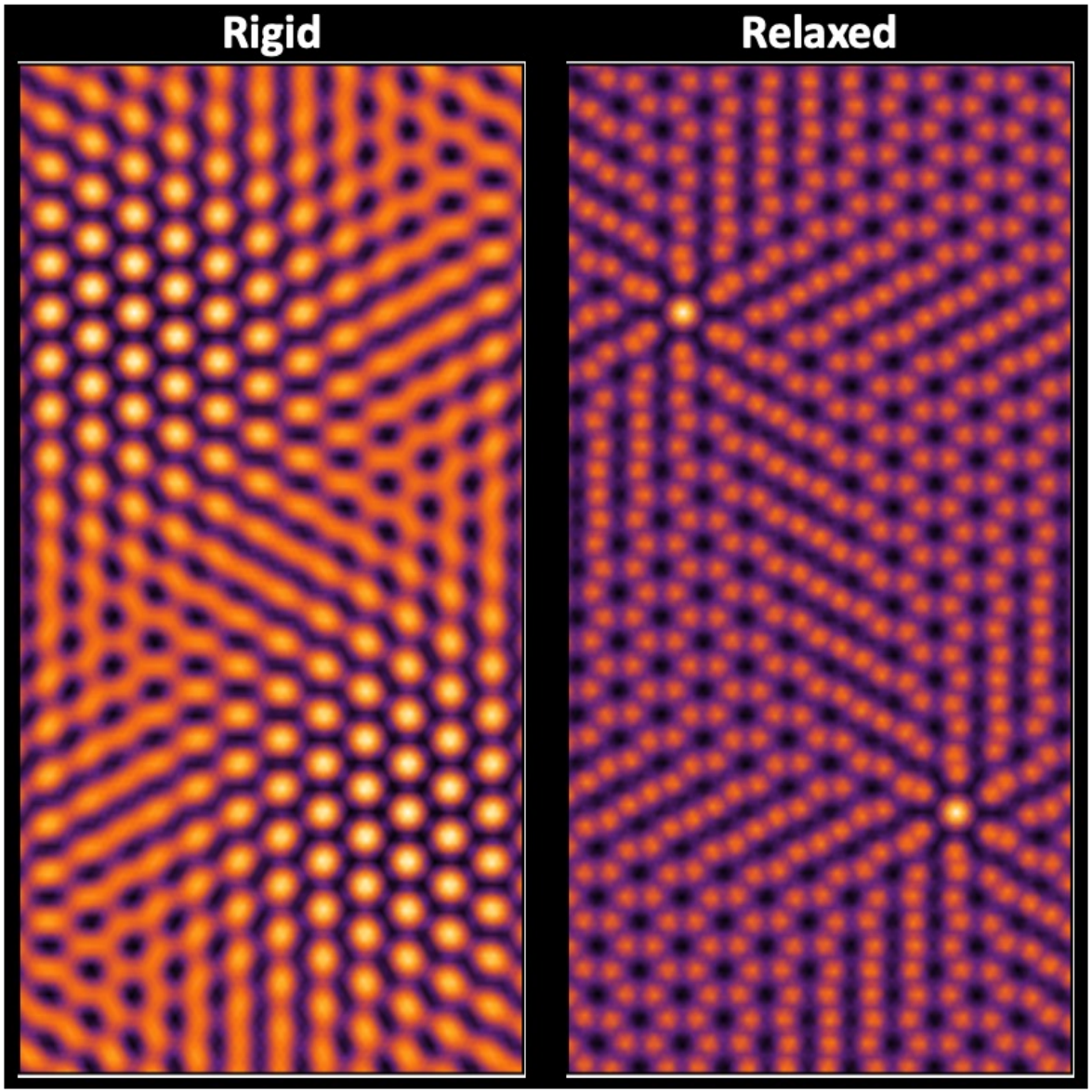
Twisted trilayer graphene (TTG)

Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.



Lattice relaxation in TTG

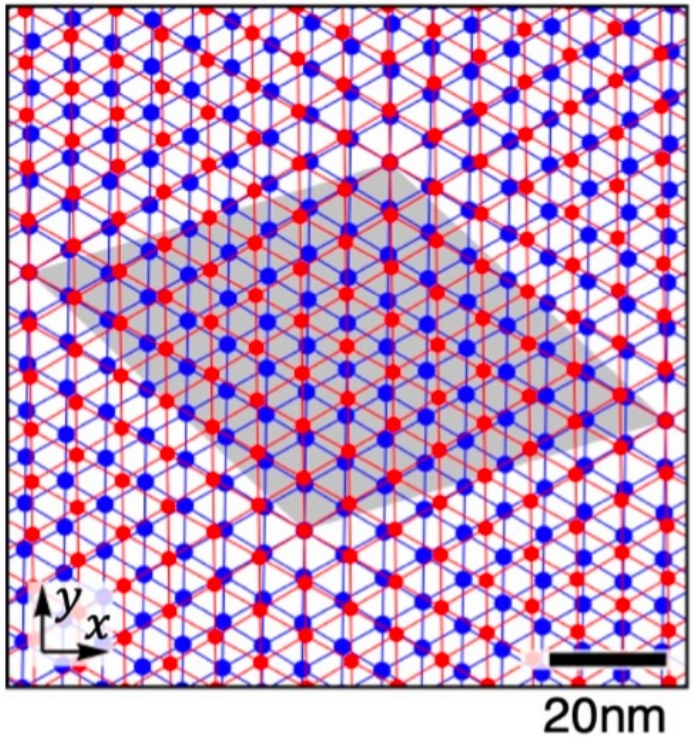
Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.



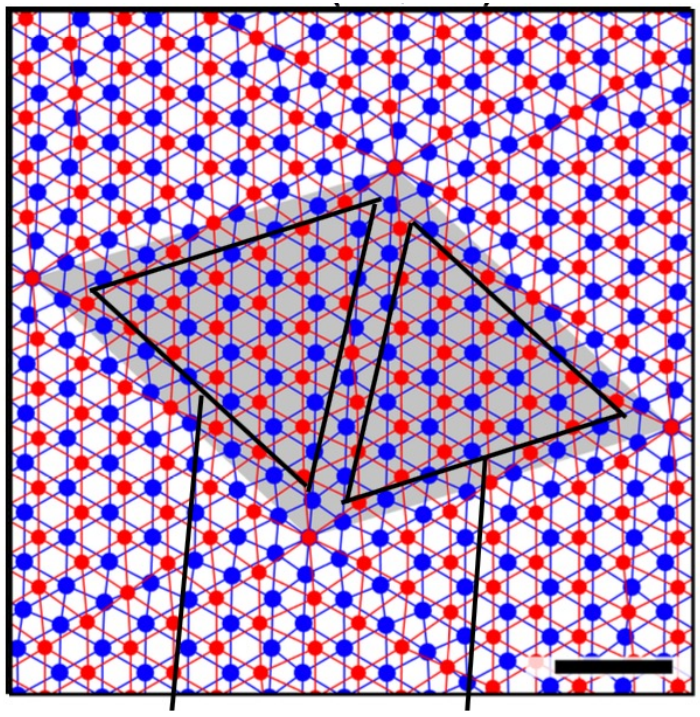
Lattice relaxation in TTG

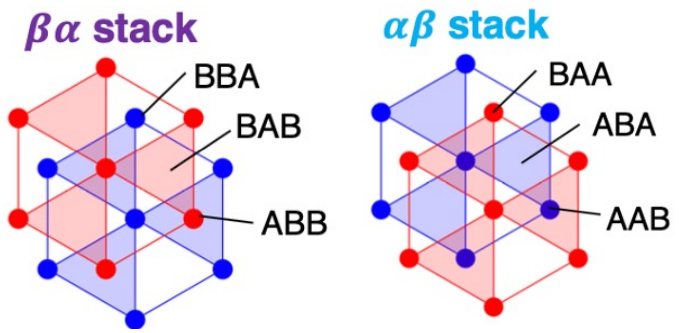
Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.

$(\theta^{12}, \theta^{23}) = (1.79°,\ 1.58°)$



relaxation



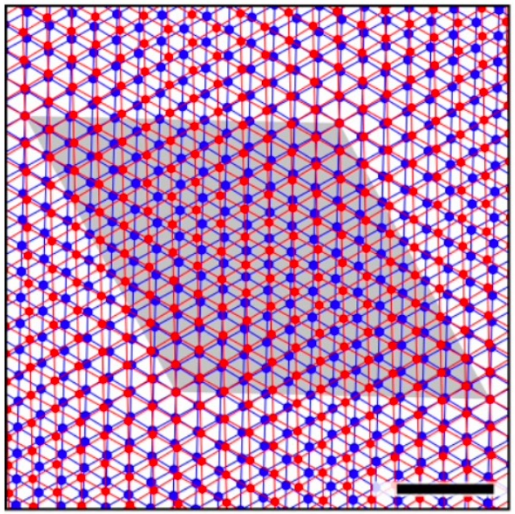


AA spots (● & ●) avoid each other
--> patchwork of commensurate super-moiré domains

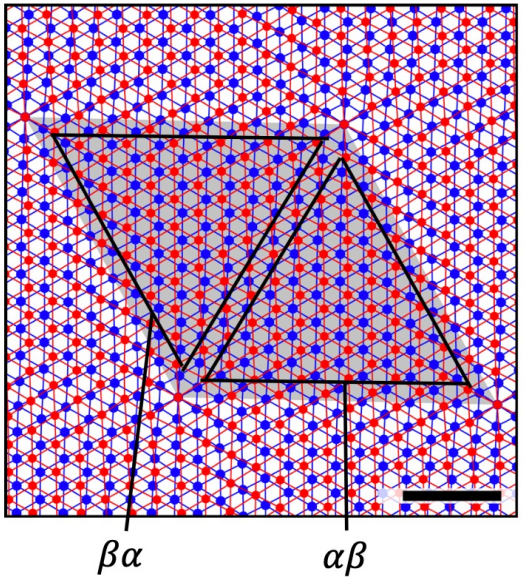
Lattice relaxation in TTG

Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.

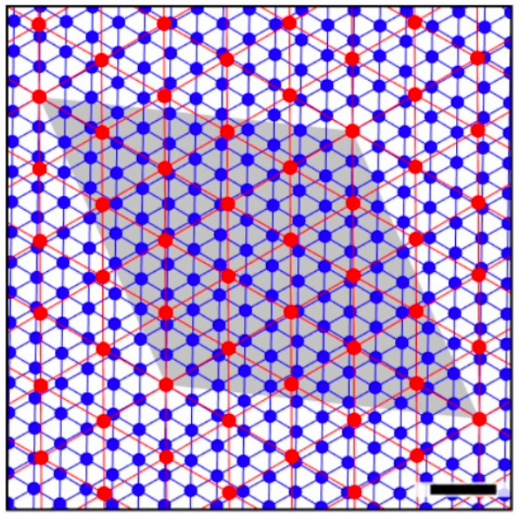
C2 $(\theta^{12}, \theta^{23}) = (2.64°,\ 2.45°)$

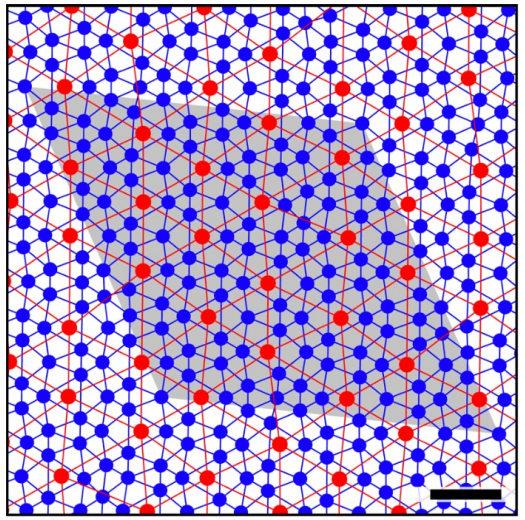


relaxation



C3 $(\theta^{12}, \theta^{23}) = (1.54°,\ 0.64°)$

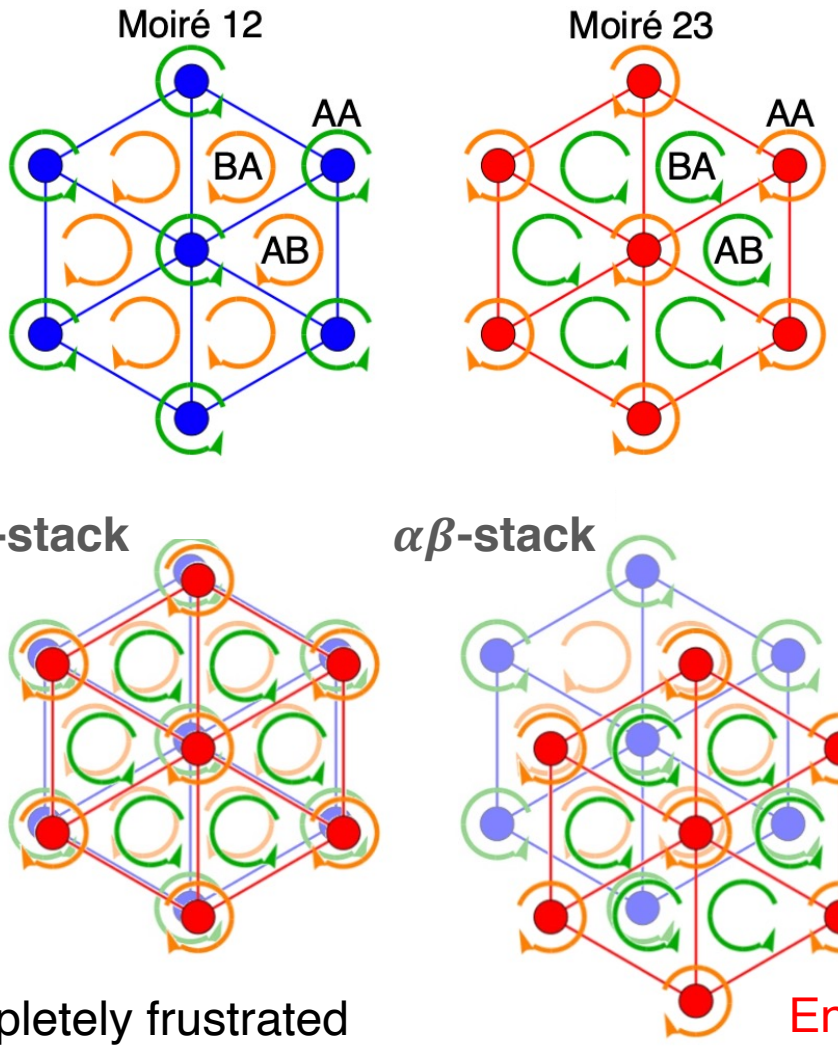




Why are the domains favored?

Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.

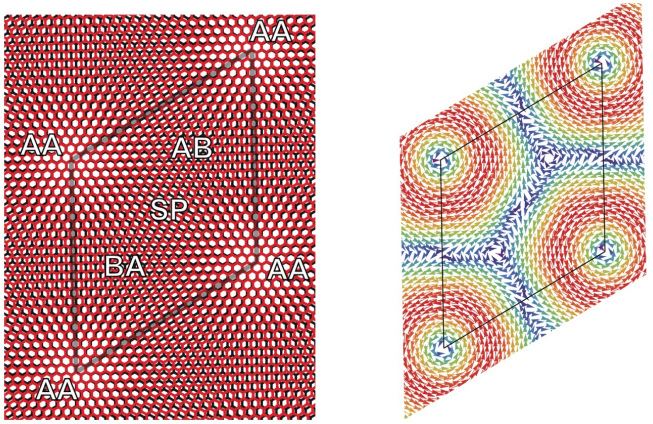
Preferred rotation direction of the middle layer



Completely frustrated

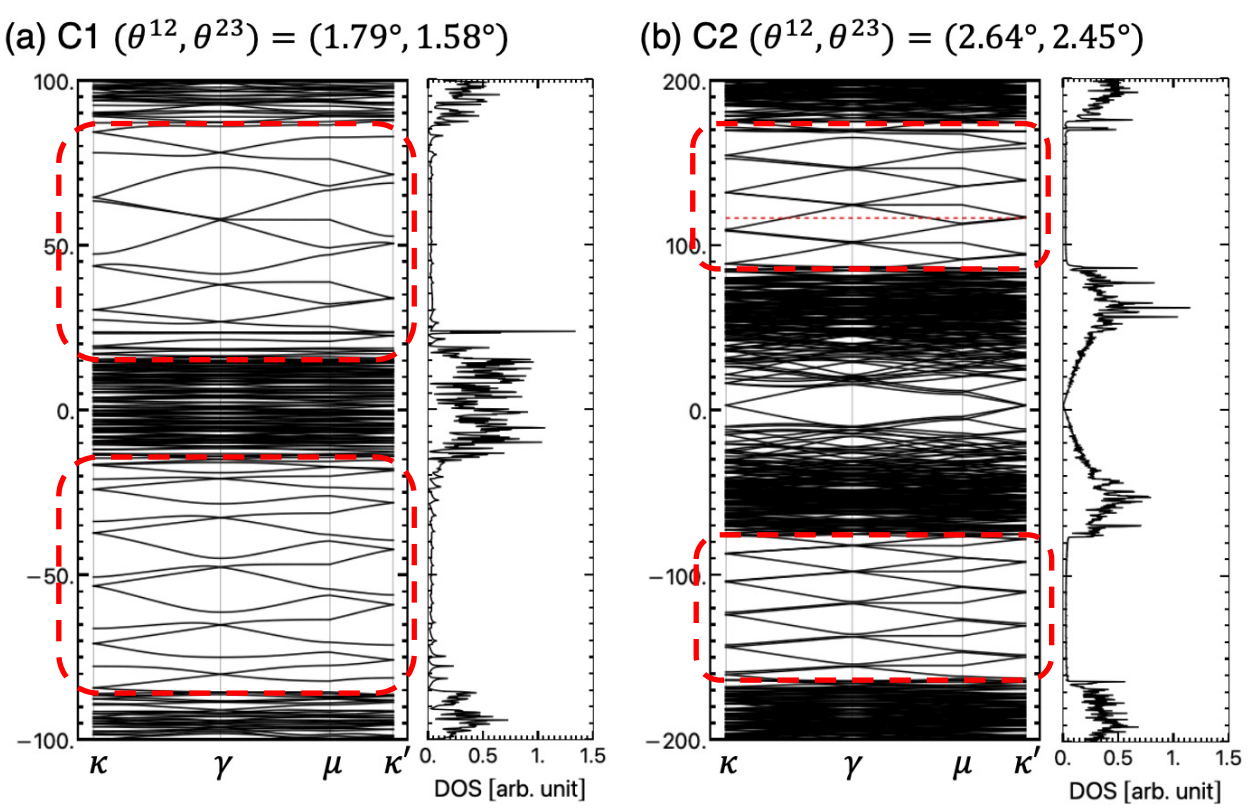
Energetically favorable !

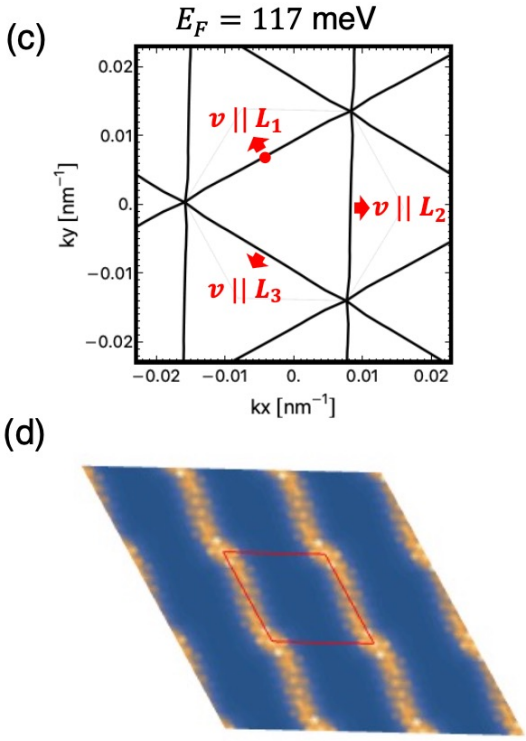
Cf. twisted bilayer graphene



Electronic structure of TTG

Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.

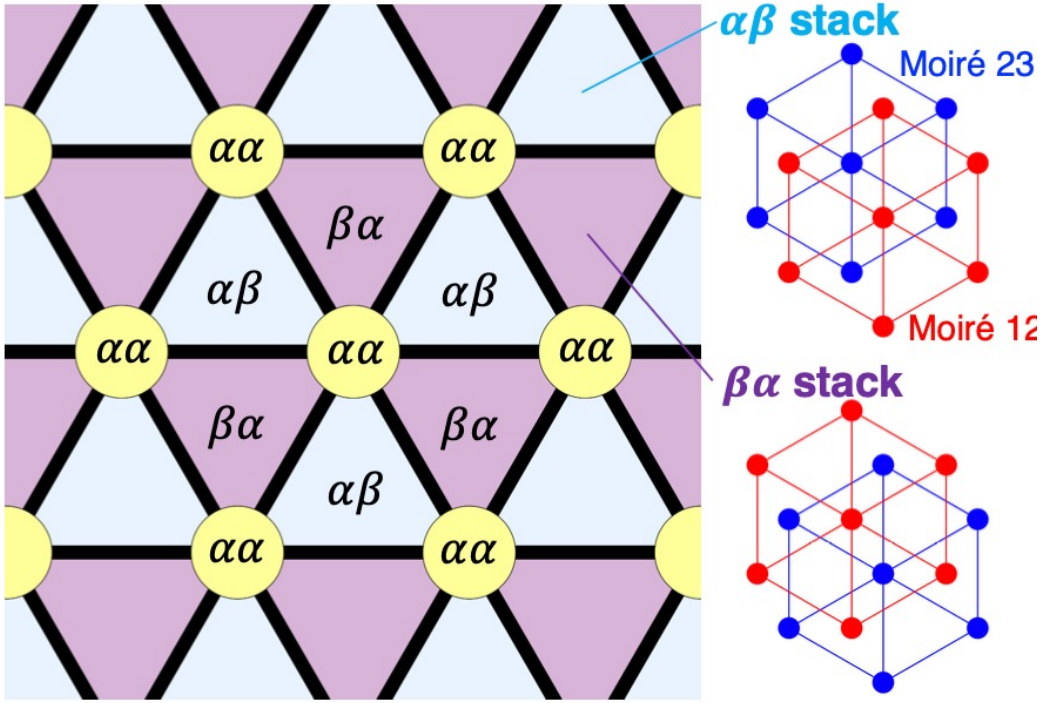


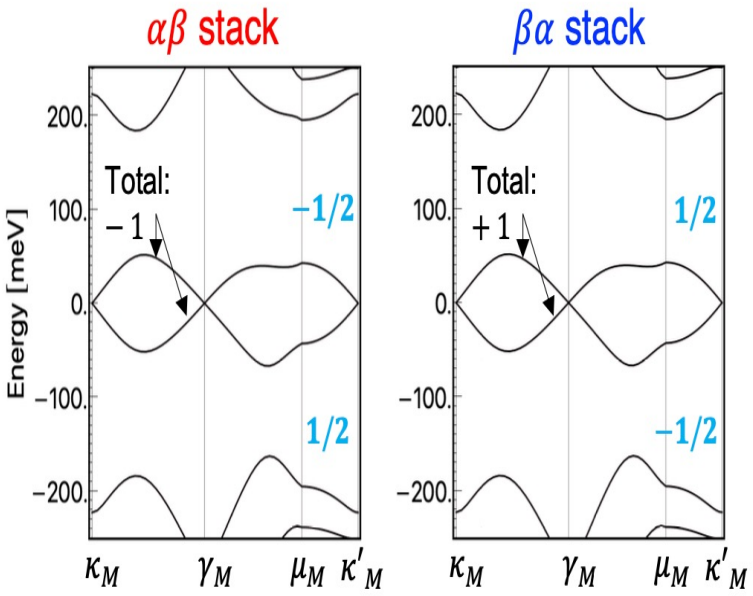


Energy window with low DOS featuring 1D electron bands

Topological domain-wall mode

Nakatsuji, Kawakami and Koshino,
arXiv:2305.13155; Phys. Rev. X, in press.

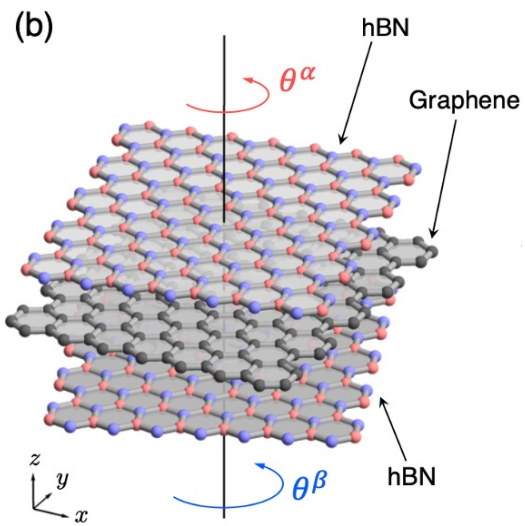


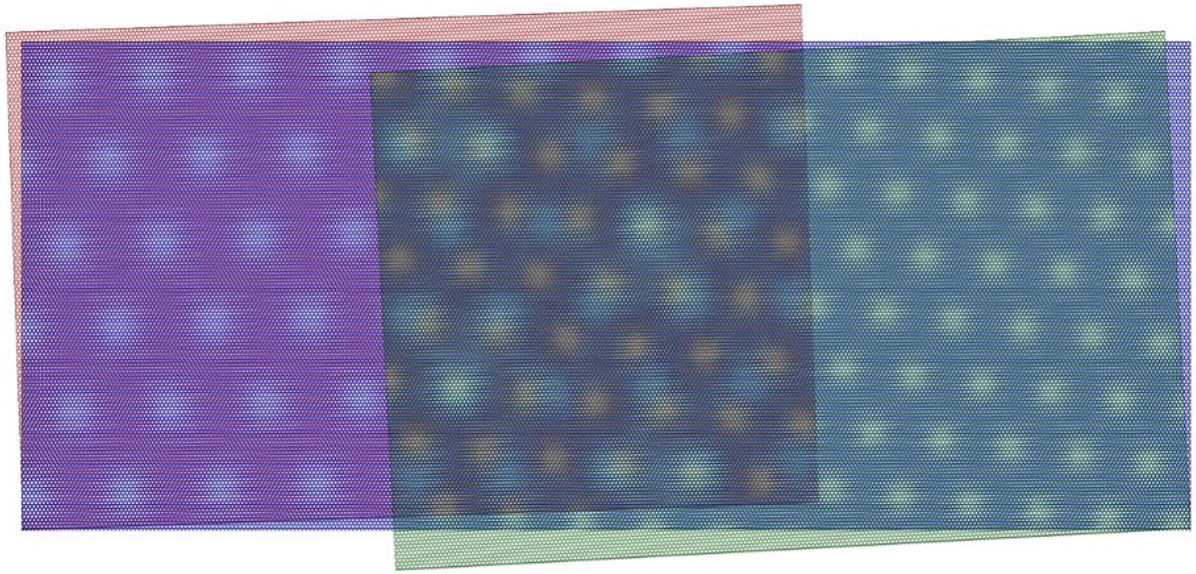


1D bands = Topological boundary states between distinct Chern insulators (valley Hall insulators)

Topological gap labeling in moiré trilayers

hBN / graphene / hBN trilayer





Double moiré pattern

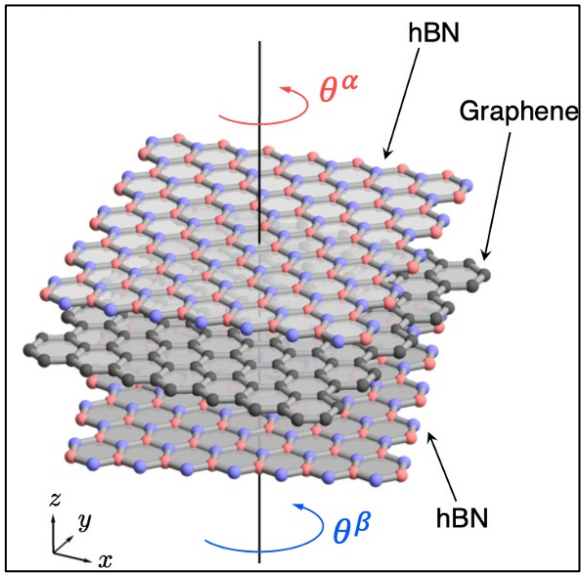
Experiment:
N. R. Finney et al,
Nat. Nanotechnol. 14, 1029 (2019).
L. Wang, et al, Nano Lett. 19, 2371 (2019).
Z. Wang, et al., Sci. Adv. 5, eaay8897 (2019).
Y. Yang, et al., Sci. Adv. 6, eabd3655 (2020).

Theory:
Andelkovic, et al,
Nano Lett. 20, 979 (2020).
Leconte and J. Jung,
2D Mater. 7, 031005 (2020).
Oka and Koshino,
Phys. Rev. B 104, 035306 (2021).

Energy spectrum of BN / graphene / BN

Oka and Koshino,
Phys. Rev. B 104, 035306 (2021).

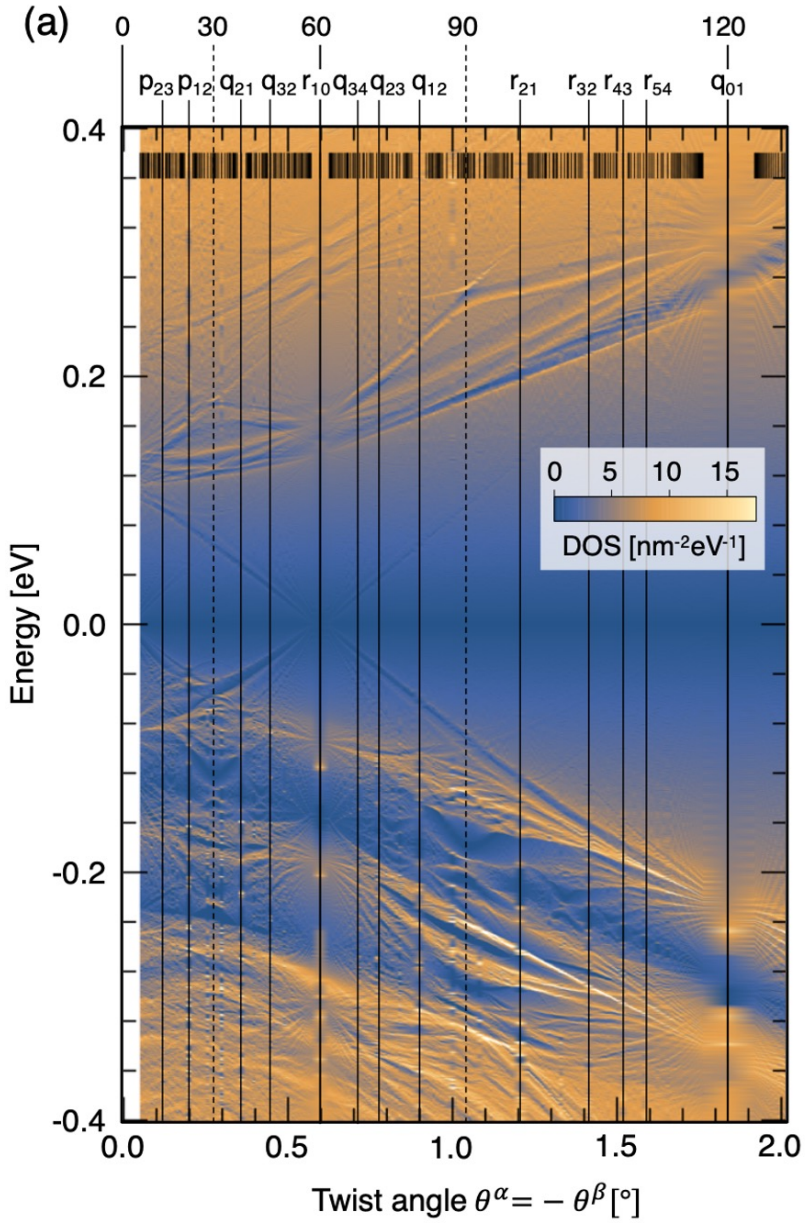
$$(\theta^\alpha, \theta^\beta) = (\theta, -\theta)$$



Interference of the two periodicities

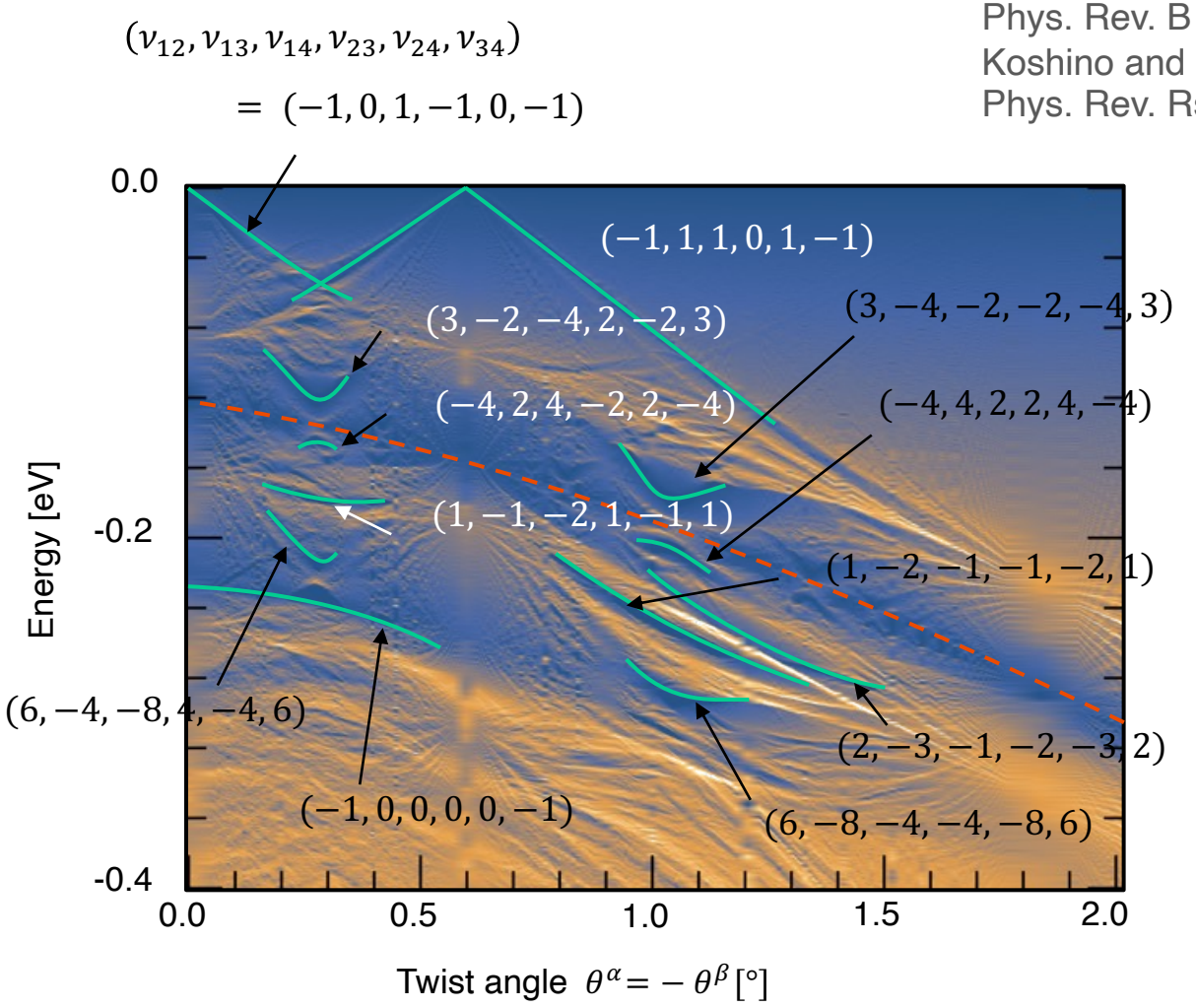
→ **fractal gap structure**
like Hofstadter's butterfly

→ **Any topologial characterization for energy gaps??**



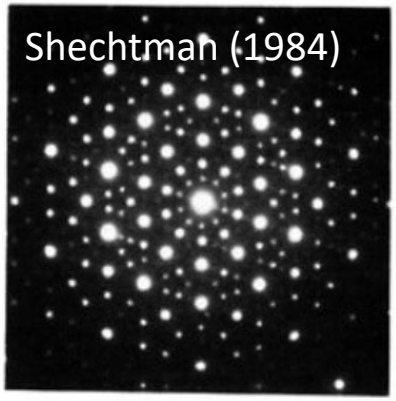
Topological numbers for energy gaps

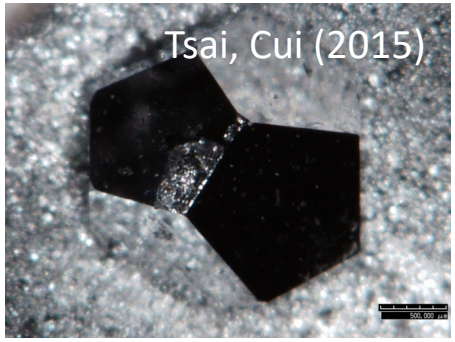
Oka and Koshino,
Phys. Rev. B 104, 035306 (2021);
Koshino and Oka,
Phys. Rev. Rsearch 4, 013028 (2022)



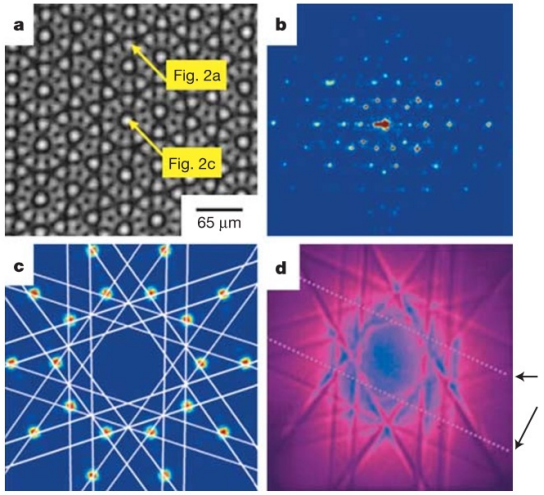
Quasicrystals

Alloy quasicrystals





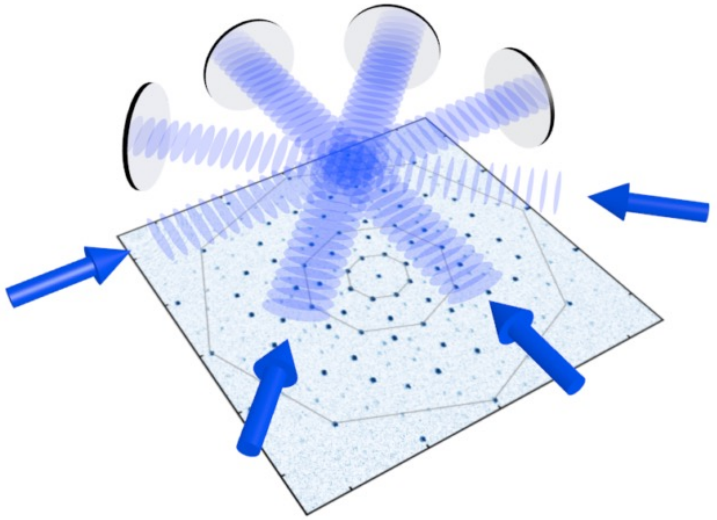
Photonic quasicrystals

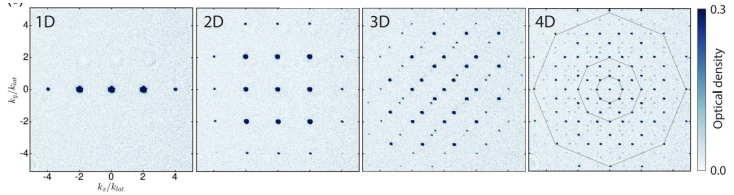


Freedman et al, Nature 440, 1166 (2006)

Cold-atom optical lattice

Viebahn et al, Phys. Rev. Lett. 122, 110404 (2019)

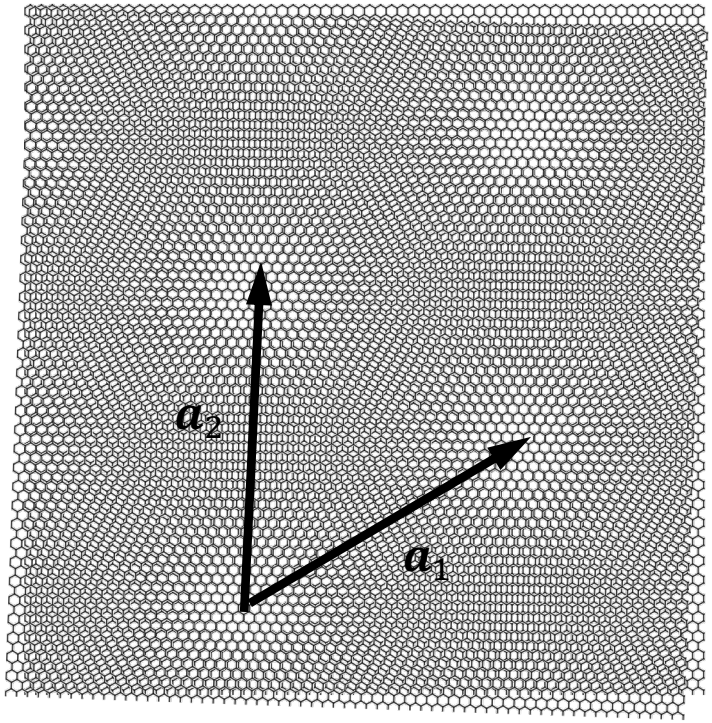




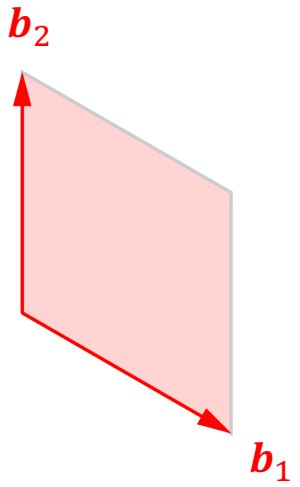
Quasicrystals =
Redundant lattice vectors
more than the spatial dimension

Single moiré system ≈ crystal (periodic)

Real space

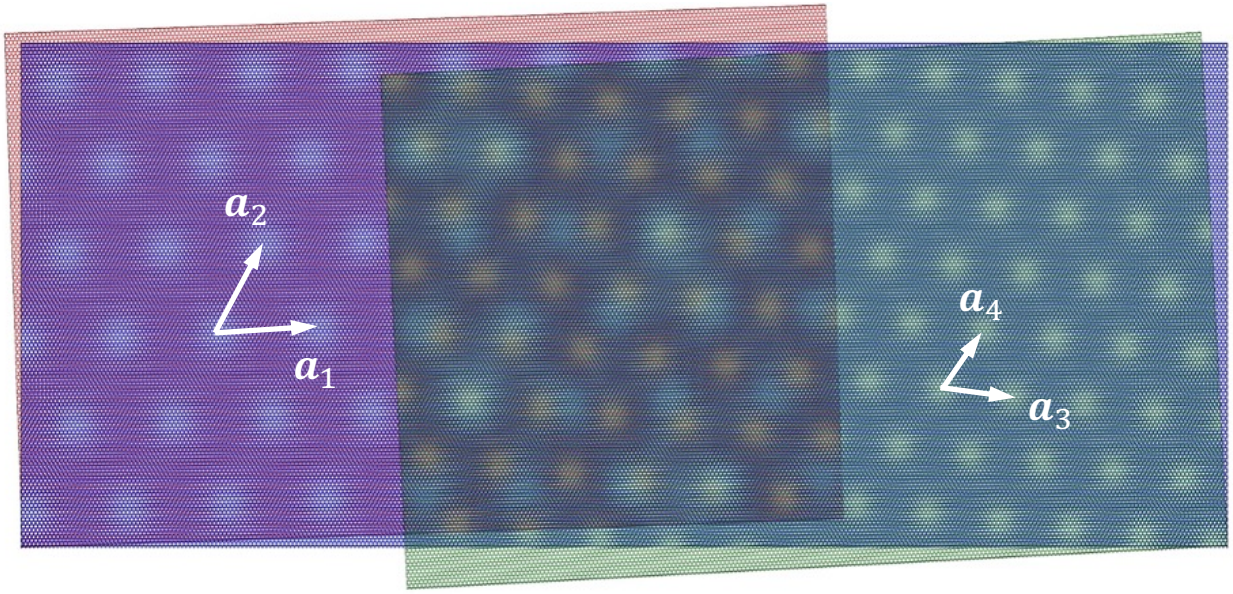


k-space
(Brillouin zone)

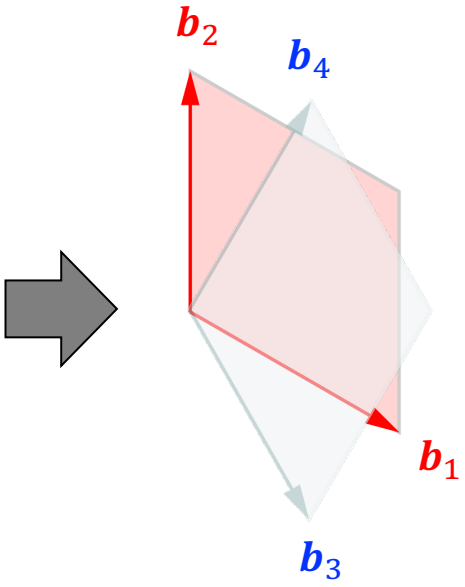


Double moiré system = **quasicrystal**

Real space



k-space
(Brillouin zone)



Redundant lattice vectors
more than the spatial dimension

→ **“moiré quasicrystal”**

Topological gap labeling in quasicrystals

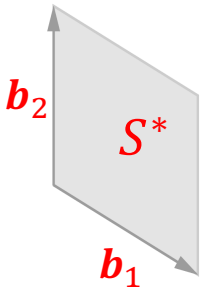
Oka and Koshino,
Phys. Rev. B 104, 035306 (2021).
Koshino and Oka,
Phys. Rev. Res. 4, 013028 (2022)

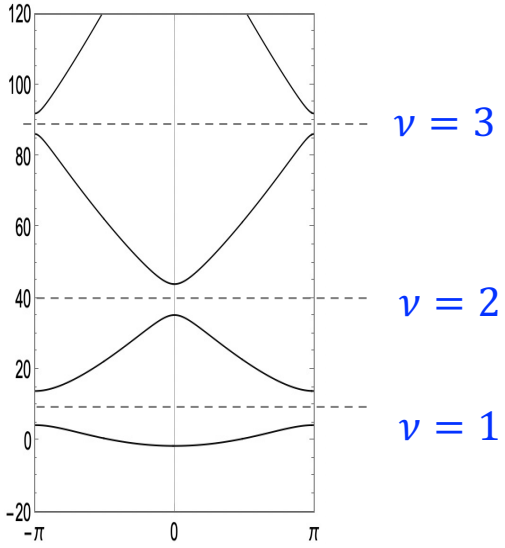
Periodic system

$$n_e = \frac{1}{(2\pi)^2}\nu S^*$$

Brillouin zone area
$\boldsymbol{b_1}\times\boldsymbol{b_2}$

Integer
(# of occupied bands)



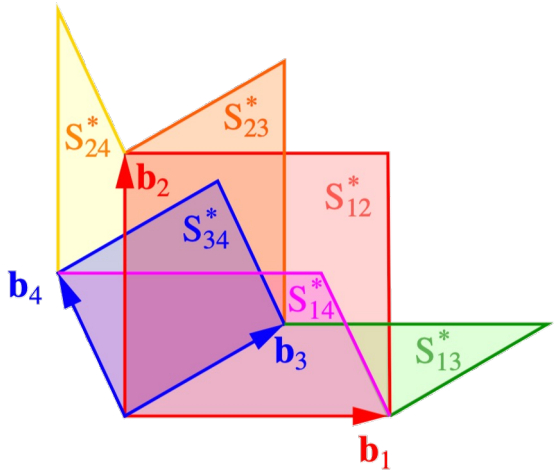


Quasiperiodic system

$$n_e = \frac{1}{(2\pi)^2}\sum_{ij}\nu_{ij}S_{ij}^*$$

Brillouin zone area
$\boldsymbol{b_i}\times\boldsymbol{b_j}$

Integer



Multiple Brillouin zones

$(i,j) = (1,2)(1,3)(1,4)(2,3)(2,4)(3,4)$

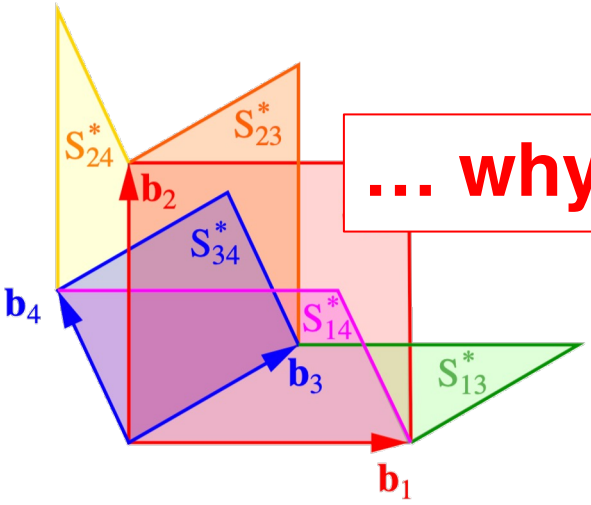
Topological gap labeling in hBN / graphene / hBN

Quasiperiodic system

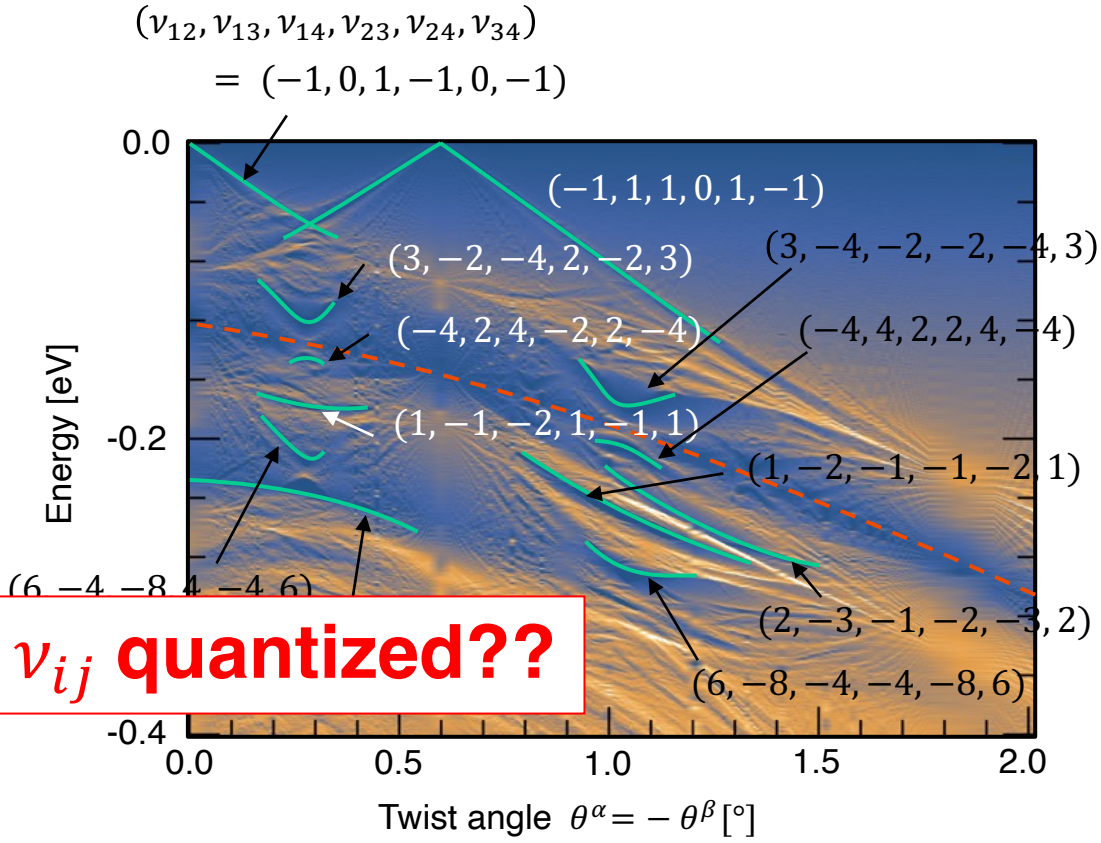
$$n_e = \frac{1}{(2\pi)^2} \sum_{ij} \nu_{ij} S_{ij}^*$$

Integer

Brillouin zone area



… why is ν_{ij} quantized??



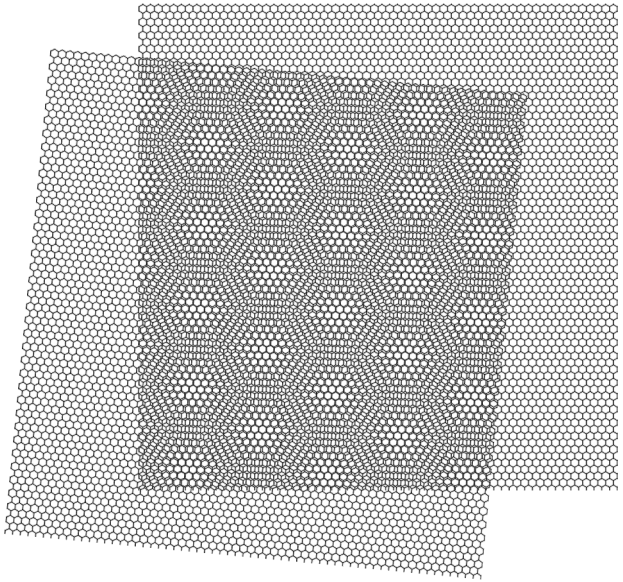
Oka and Koshino,
Phys. Rev. B 104, 035306 (2021);
Koshino and Oka,
Phys. Rev. Rsearch 4, 013028 (2022)

ν_{ij} = a second Chern number

Koshino and Oka,
Phys. Rev. Research
4, 013028 (2022)

Adiabatic pumping in interlayer sliding

M. Fujimoto, H. Koschke, and M. Koshino,
Phys. Rev. B 101, 041112 (2020).



Dimensional reduction

movement of moiré pattern
→ **charge current**

… quantized by ν_{ij}

4D Quantum Hall effect

Electromagnetic response

$$j_\mu^{(4D)} = \frac{e^3}{h^2} C^{(2)} \epsilon^{\mu\nu\lambda\rho} B_{\nu\lambda} E_\rho$$

Second Chern number

$$C^{(2)} = \frac{1}{4\pi^2} \int_{BZ} d^4k \, (F^{xy}F^{zw} + F^{xw}F^{zy} + F^{zx}F^{wy})$$

$$F^{\mu\nu} = i[\langle \partial_\mu u | \partial_\nu u \rangle - \langle \partial_\nu u | \partial_\mu u \rangle]$$

X.-L. Qi, T. L. Hughes, and S.-C. Zhang,
Phys. Rev. B 78, 195424 (2008).
Y. E. Kraus, Z. Ringel, and O. Zilberberg,
Phys. Rev. Lett. 111, 226401 (2013).

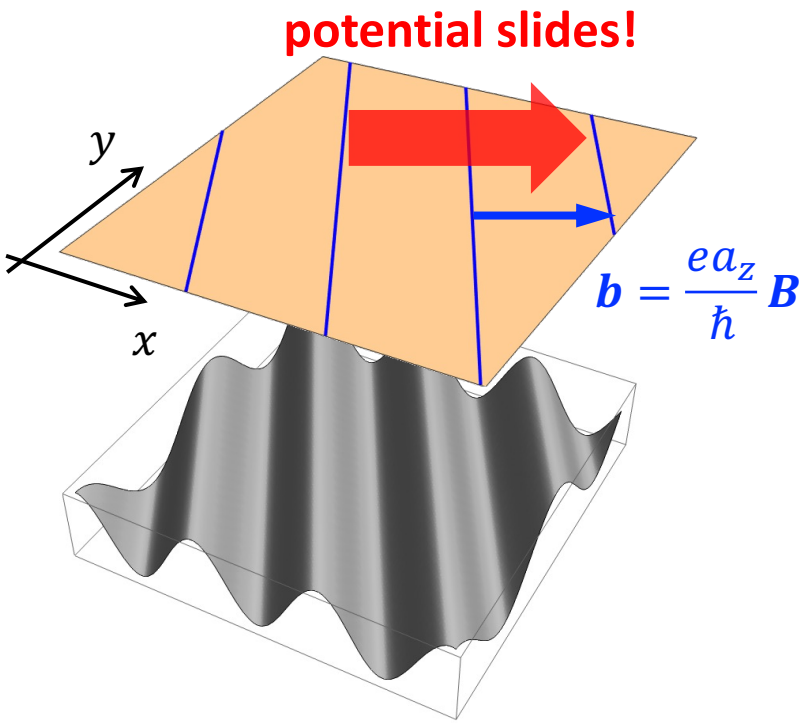
Cf. First Chern number: $C^{(1)} = \frac{1}{2\pi} \int_{BZ} d^2k \; F^{xy}$

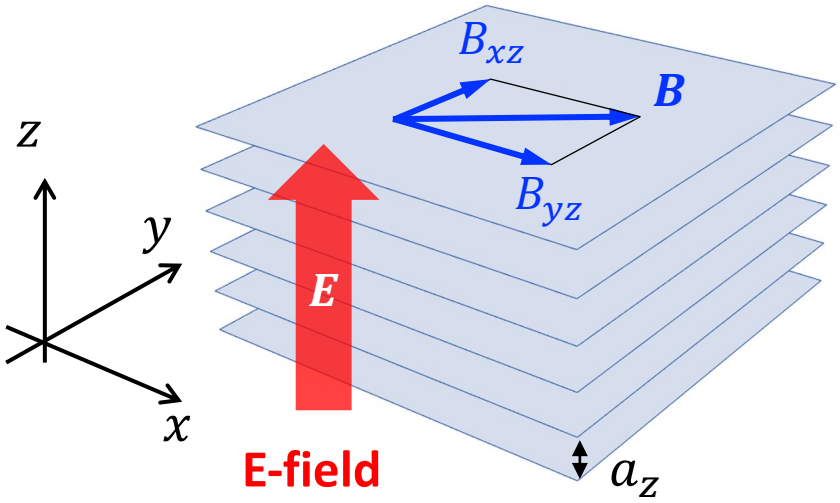
Mapping to higher-dimensional system

Koshino and Oka,
Phys. Rev. Research
4, 013028 (2022)

2D system + a periodic potential

3D system + B field





Adiabatic pumping

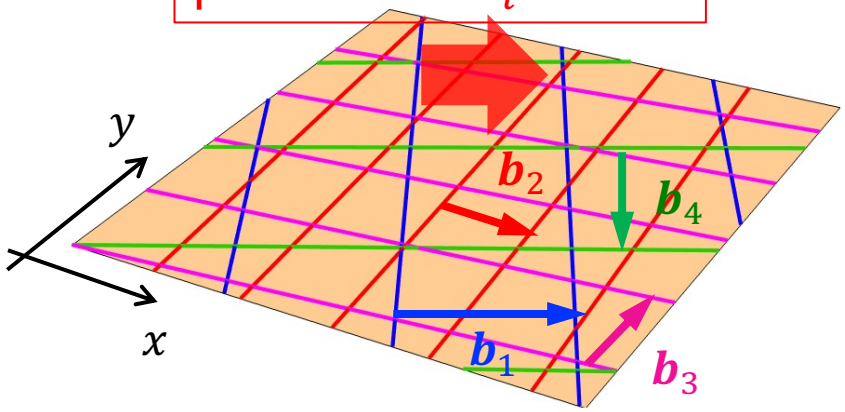
Quantum Hall effect

Mapping to higher-dimensional system

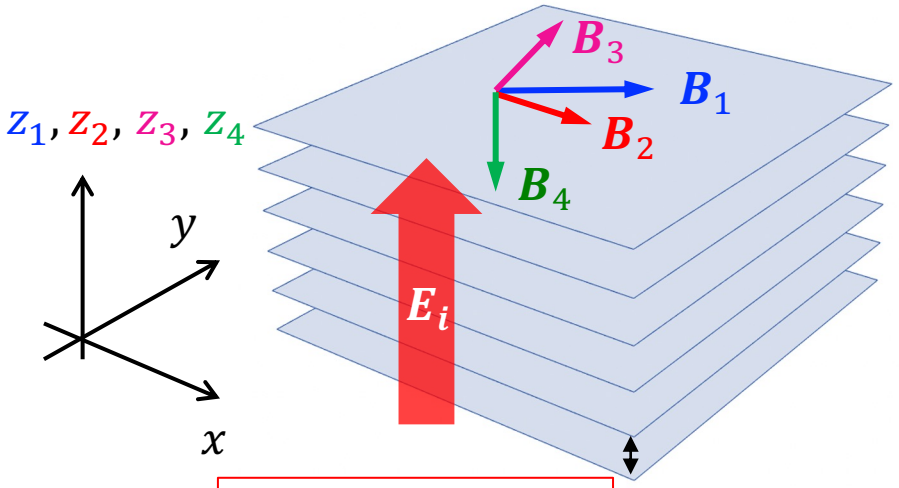
Koshino and Oka,
Phys. Rev. Research
4, 013028 (2022)

2D system + 4 periodic potentials ⟷ **6D system + B field**

potential of $\boldsymbol{b}_i$ slides



$$\boldsymbol{B}_i = (B_{xi}, B_{yi})\ (i = 1,2,3,4)$$



E-field along z_i

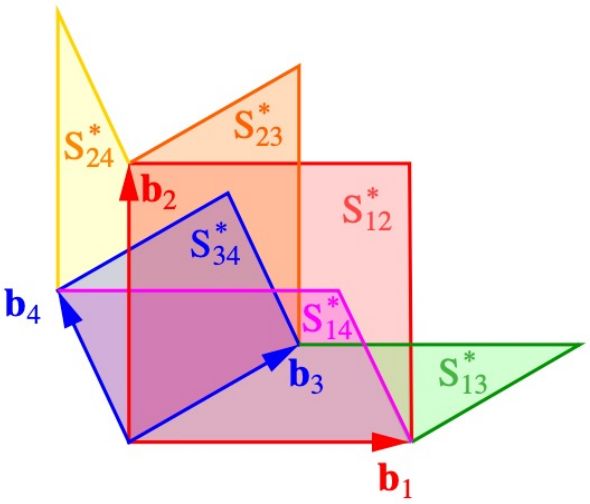
a_1, a_2, a_3, a_4

Adiabatic pumping ⟷ Quantum Hall effect

Physical meaning of ν_{ij}

Koshino and Oka,
Phys. Rev. Research 4, 013028 (2022)

k-space

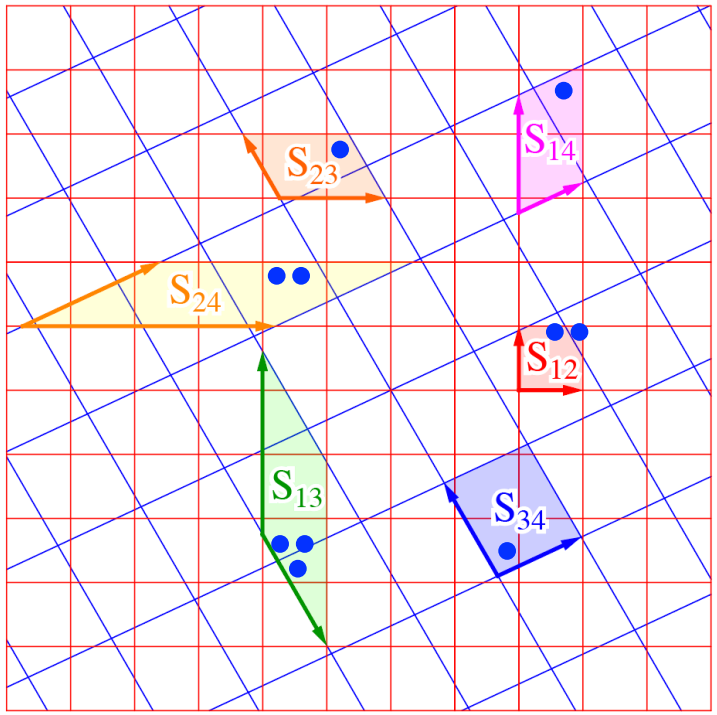


$$n_e = \frac{1}{(2\pi)^2}\sum_{ij} \nu_{ij} S^*_{ij}$$

Real space unit cell

$$S_{ij} = \frac{(2\pi)^2}{S^*_{ij}}$$

r-space



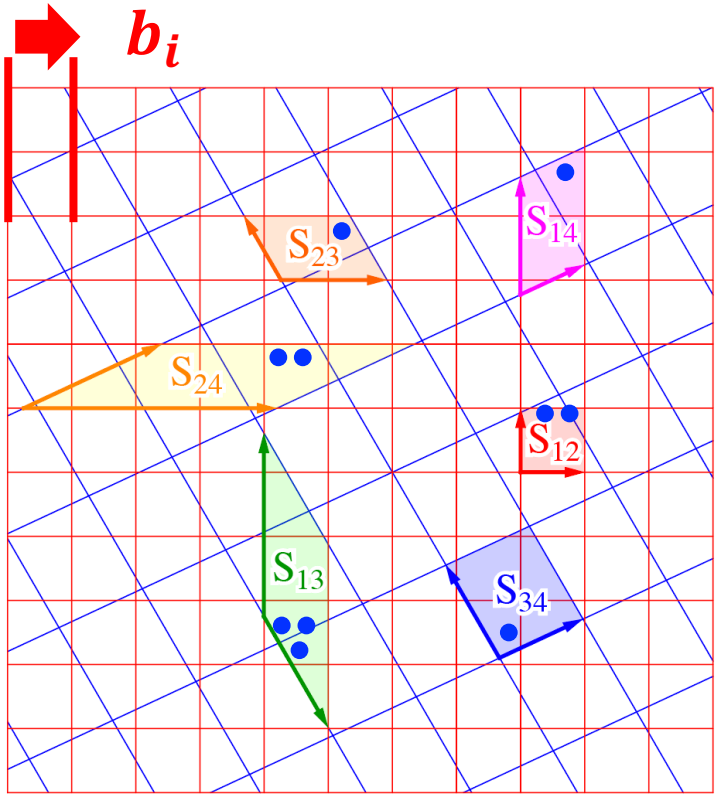
$$n_e = \sum_{ij} \frac{\nu_{ij}}{S_{ij}}$$

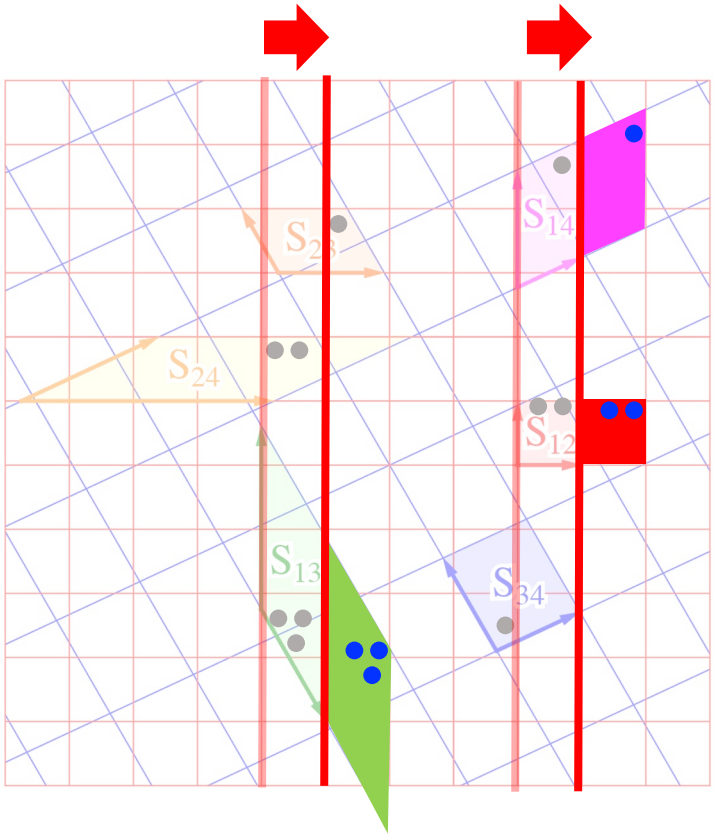
ν_{ij} electrons reside in every unit cell of S_{ij}

Adiabatic charge pumping

Koshino and Oka,
Phys. Rev. Research 4, 013028 (2022)

Charge pumping by sliding a single potential





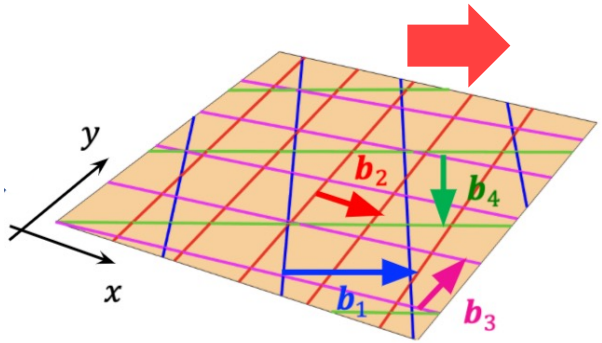
$$n_e = \sum_{ij} \frac{\nu_{ij}}{S_{ij}}$$

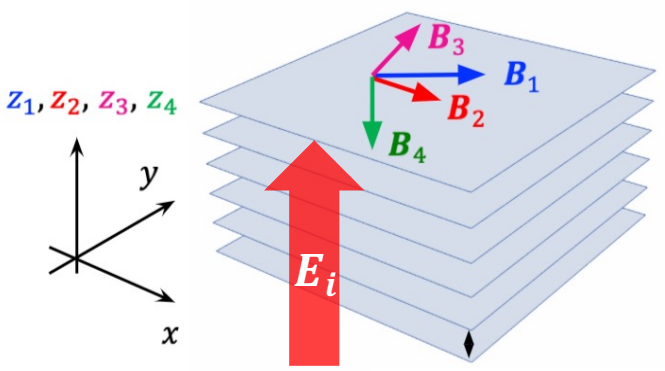
Charge shift: $$\Delta \boldsymbol{P}_i = \frac{1}{2\pi} \sum_j \nu_{ij} (\boldsymbol{b}_j \times \boldsymbol{e}_z)$$

Mapping to a high-dimensional system

Koshino and Oka,
Phys. Rev. Research 4,
013028 (2022)

2D quasi-periodic system ⟷ **6D system + B field**





Adiabatic charge pumping
in potential sliding

Electromagnetic response
in (x, y, z_i, z_j) -subspace **(4D QHE)**

$$\Delta \boldsymbol{P}_i = \frac{1}{2\pi}\sum_j \boxed{\nu_{ij}}(\boldsymbol{b}_j \times \boldsymbol{e}_z) \quad \longleftrightarrow \quad \boldsymbol{j}^{(4D)} = \frac{1}{4\pi^2}\boxed{C_{ij}^{(2)}} E_i(\boldsymbol{B}_j \times \boldsymbol{e}_z)$$

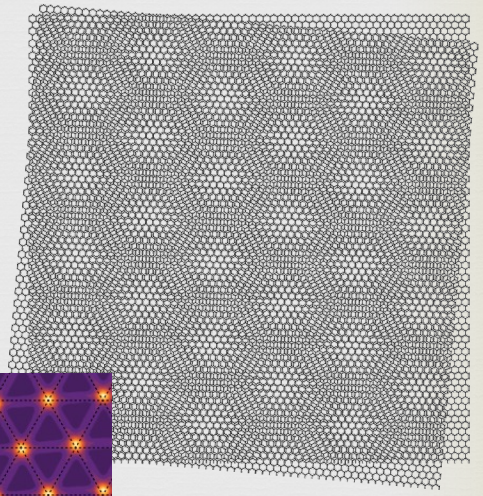
Second Chern number

Quantization of
electron density ⟵ $\nu_{ij} = C_{ij}^{(2)}$ ⟶ Quantization of
4D Hall conductivity

Summary: Physics of moiré materials & beyond

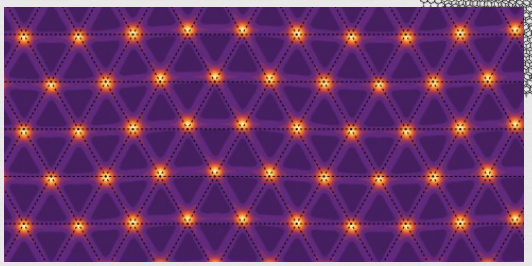
Twisted bilayer graphene

-- Moiré electron bands and continuum model



Moiré phonons

-- Vibration of “moiré atoms”



Moiré trilayer systems

-- Moiré-of-moiré domain

-- Topological gap labelling with 2nd Chern number