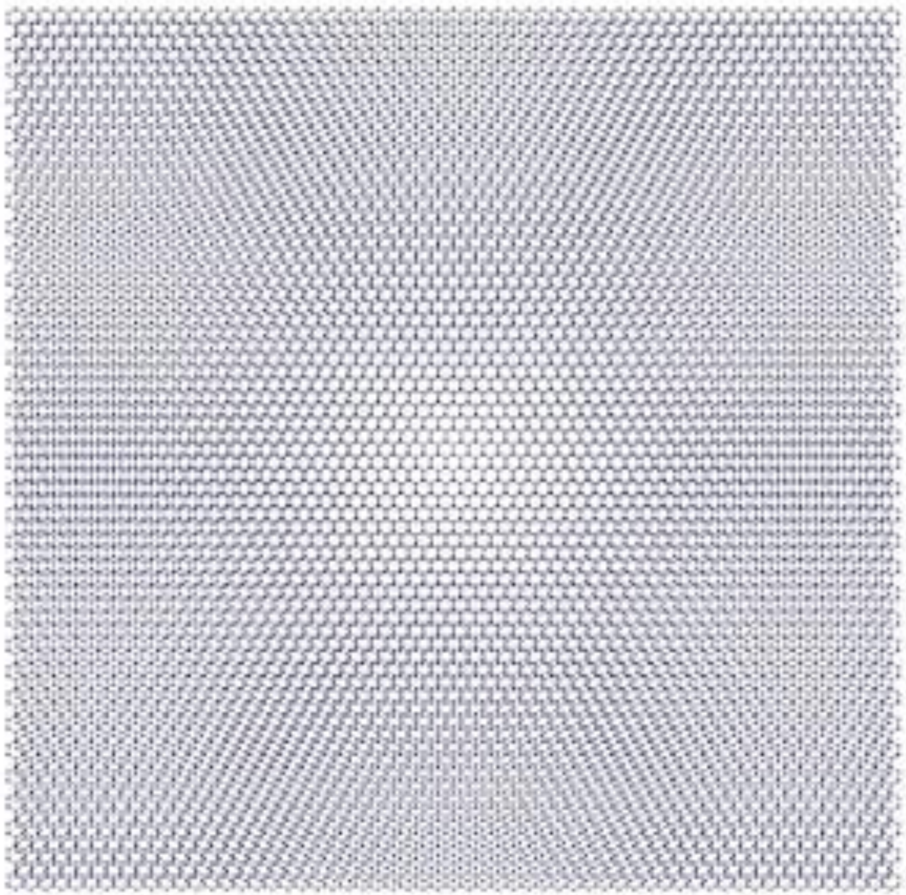

Magic-angle twisted 2D materials

Group Member: 王杏 林益浩 王昊 杜思敬 赵天伦 李科卫 王继鹏

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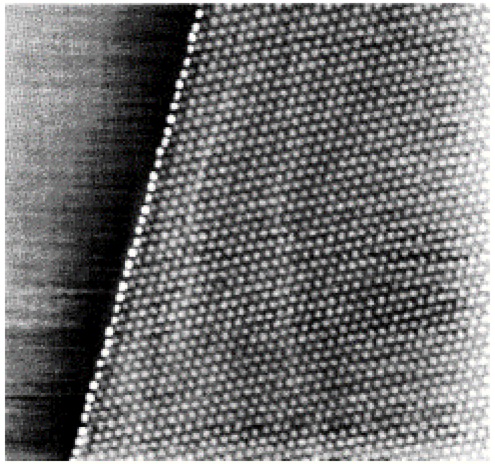
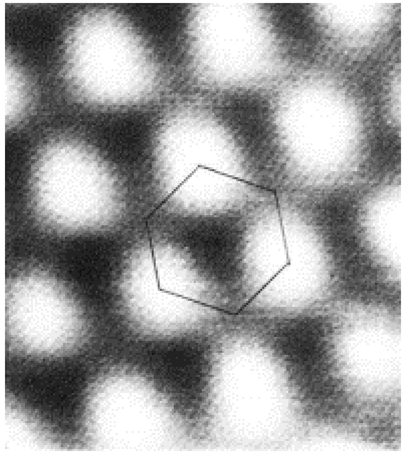
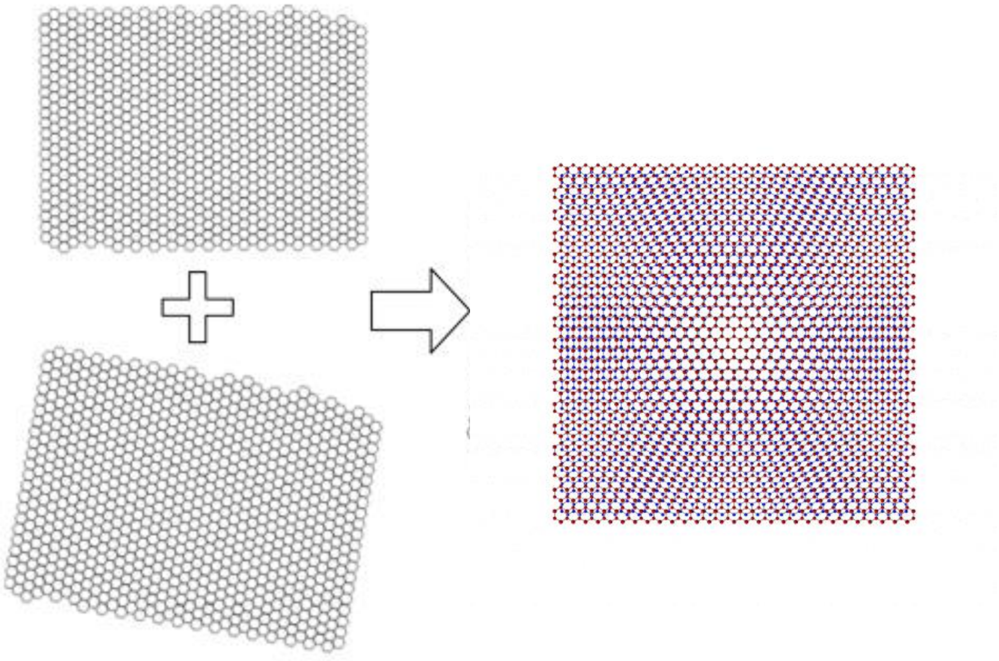
- Moire Pattern & Twistronics
- Moire band and Magic angle
- Experiments
- Summary

Moire Pattern



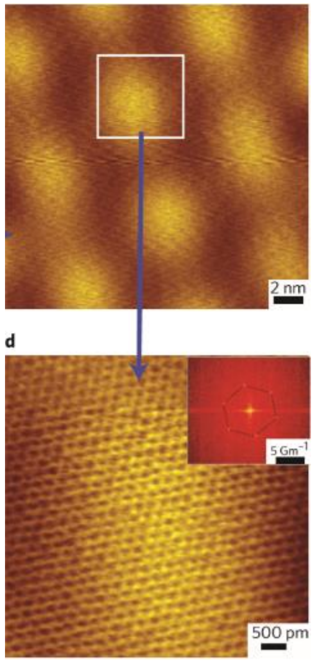


$$D = d/[2\sin(\theta/2)]$$

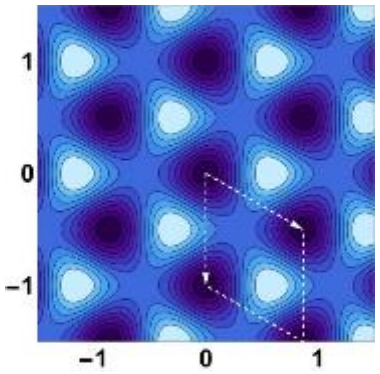


2005 Pong, W.-T., Durkan, C. J. Phys. D:Appl. Phys. 38(21), pp. R329-R355

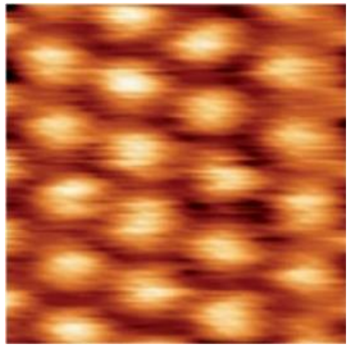
Twisted 2D materials & Twistronics



Twisted bilayer graphene



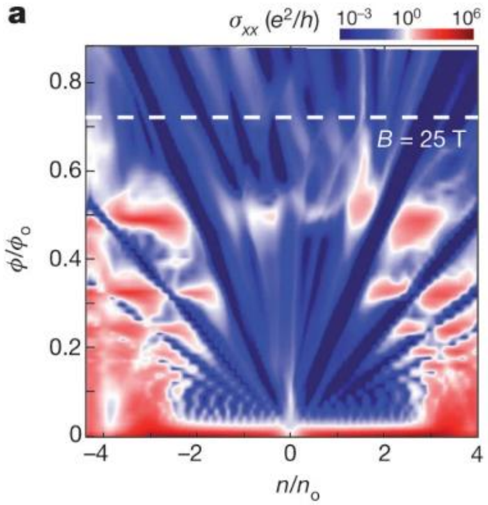
WS2/MoS2 heterobilayers



Bilayer graphene on h-BN

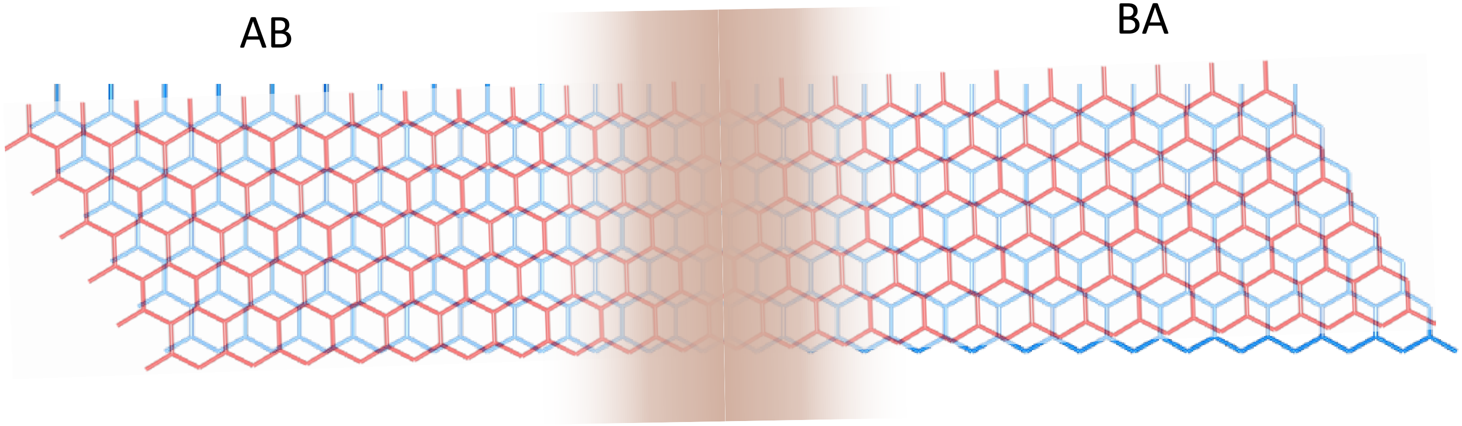
Novel Physical Properties：

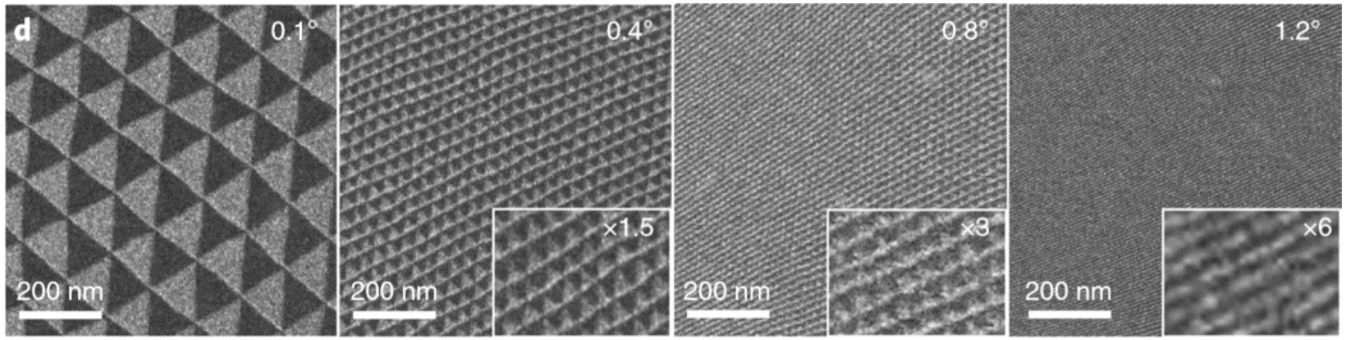
- Unconventional superconductivity
- Moire excitons
- Hofstadter's butterfly
- …



2010 Li, G.et.al. Nat. Phys. 6(2), pp. 109-113
2018 Wu, F. et.al. PRB 97(3),035306
2013 Ponomarenko, L.A.et.al. Nature 497(7451), pp. 594-597
2013 Dean, C.R. et.al. Nature. 497(7451), pp. 598-602

Twisted bilayer graphene(TBG)

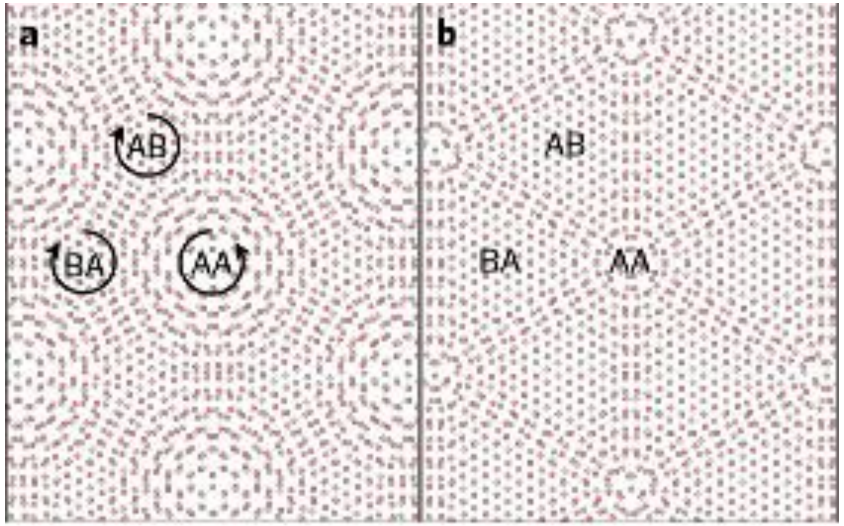




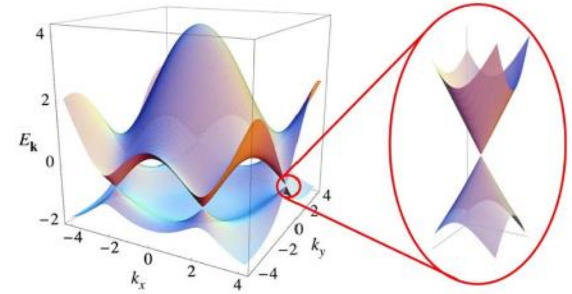
2019 Yoo, H.et.al. Nat. Mat. 18(5), pp. 448-453

Atomic and electronic reconstruction at the van der Waals interface in twisted bilayer graphene

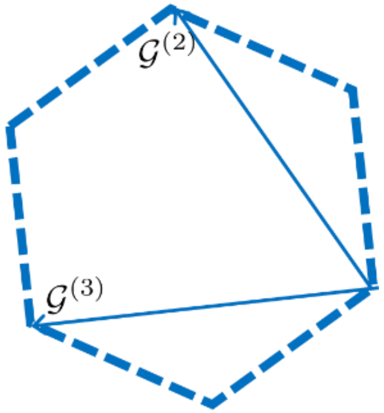
Formation of the "commensurate domains"



Contents



Moire band

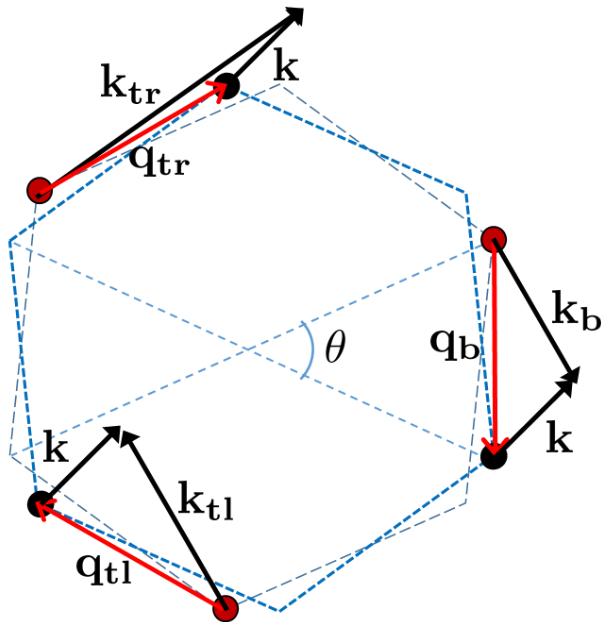


Problem:

- Breakdown of Bloch electron picture due to Incommensurate structure

Solution: Notion of Moire band

- 2011 Bistritzer, R.et.al. PNAS. *Moiré bands in twisted double-layer graphene*



$$H = \begin{pmatrix} h(-\theta/2) & T(\mathbf{r}) \\ T^{\dagger}(\mathbf{r}) & h(\theta/2) \end{pmatrix}$$

Layers' Dirac cone :

$$h = iv\sigma \cdot \nabla$$

Three types of interlayer hopping:

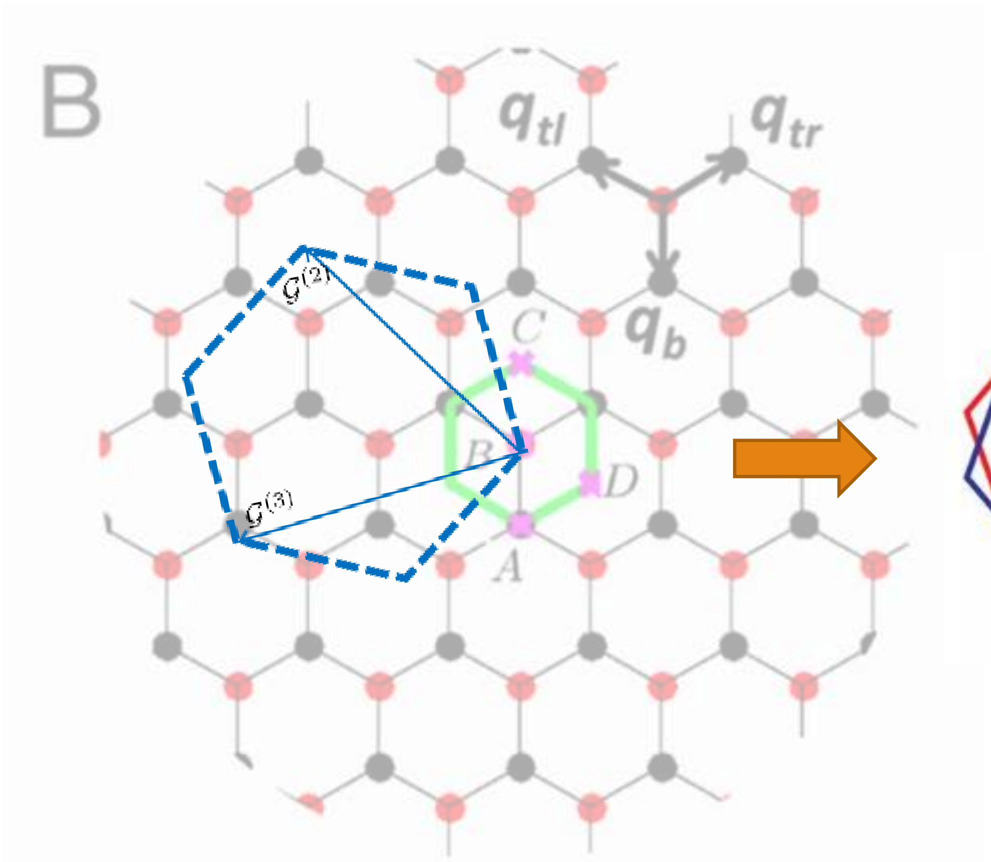
$$T(\mathbf{r}) = w \sum_j e^{-i\mathbf{q}_j \cdot \mathbf{r}} T_j$$

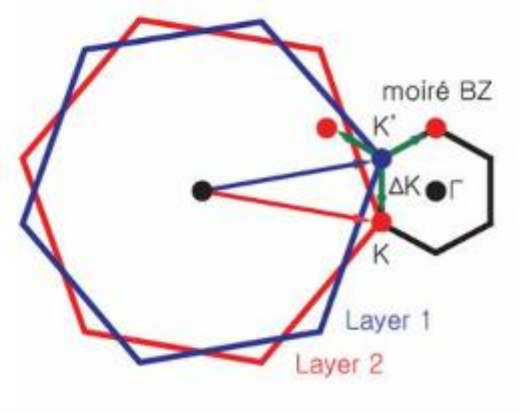
w ~ vdW interaction strength

$$T_1 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, T_2 = \begin{pmatrix} e^{-i\phi} & 1 \\ e^{i\phi} & e^{-i\phi} \end{pmatrix}, T_3 = \begin{pmatrix} e^{i\phi} & 1 \\ e^{-i\phi} & e^{i\phi} \end{pmatrix}$$

where $\phi = 2\pi/3$

Moire band





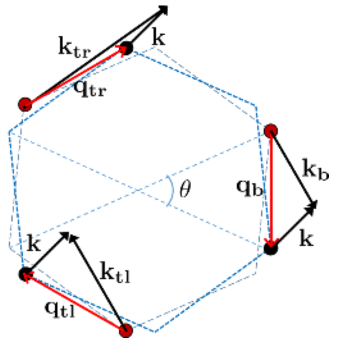
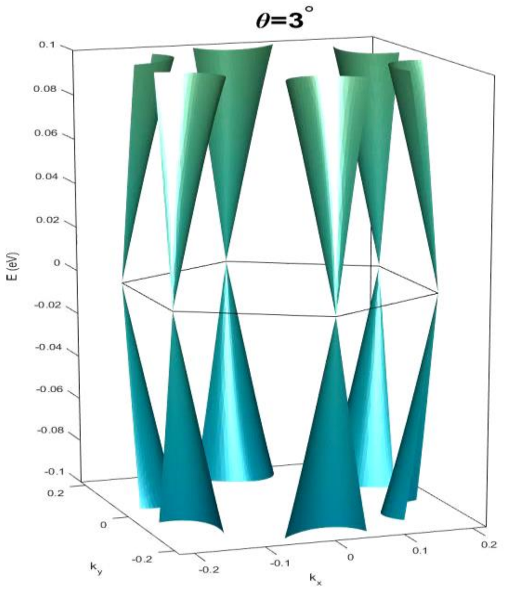
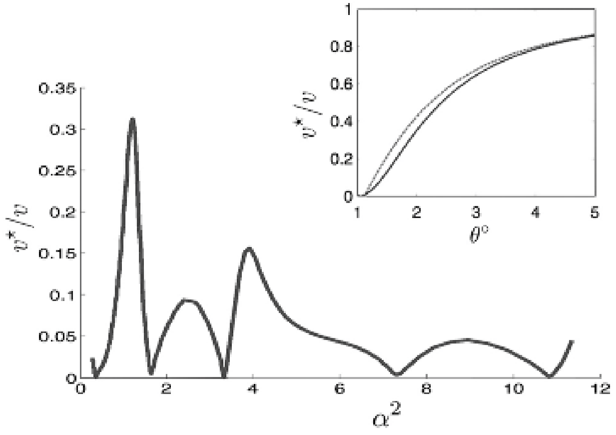


Figure from
2017 Kim, K. et.al. PNAS 114(13), pp. 3364-3369

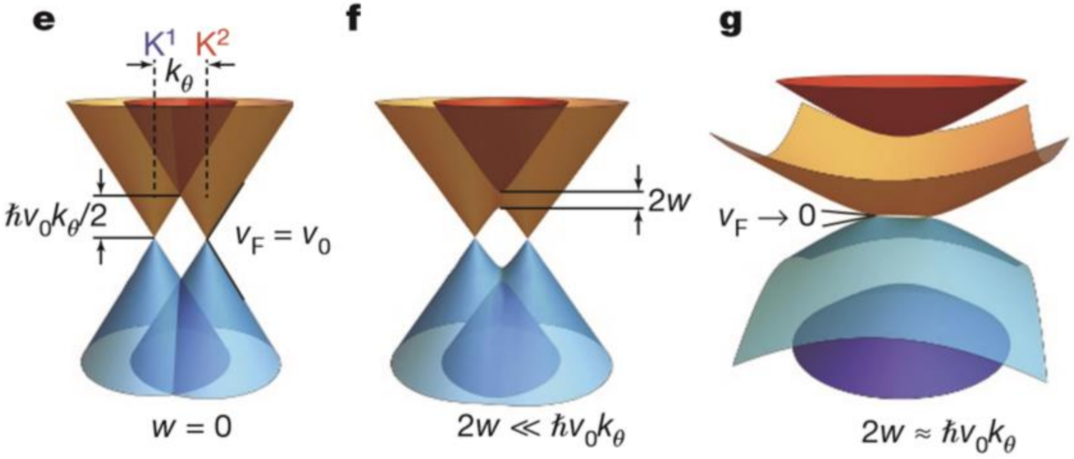
Emergence of “Magic angle”





Calculated Fermi velocity of Moire Dirac cone

$$\alpha = w/vk_\theta$$



When kinetic energy ~ interlayer vdW interaction

List of “magic angle” $\theta \approx 1.05°$, $0.5°$, $0.35°$, $0.24°$, $0.2°$

2018 Cao, Y. Nature 556(7699), pp. 80-84

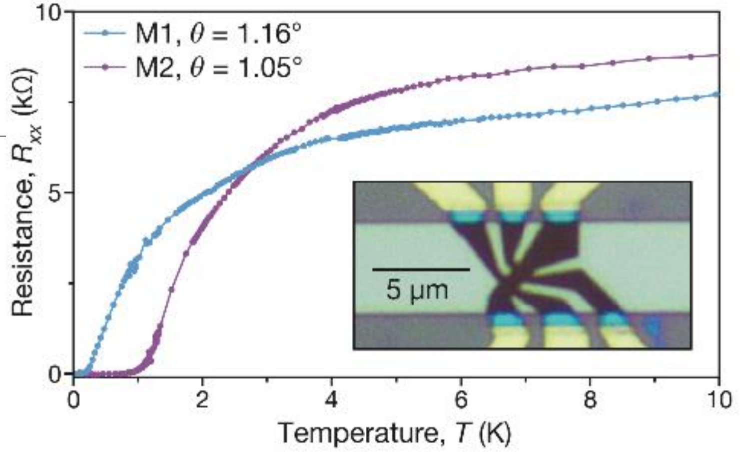
2011 Bistritzer, R.et.al. PNAS. 108(30), pp. 12233-12237 nature > articles > article

Published: 05 March 2018

Unconventional superconductivity in magic-angle graphene superlattices

Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras & Pablo Jarillo-Herrero

Nature **556**, 43–50(2018) | Cite this article



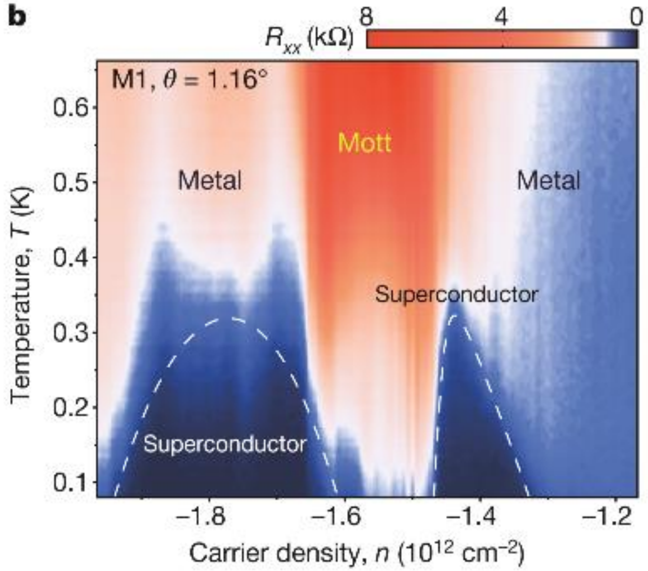
nature > letters > article

Published: 05 March 2018

Correlated insulator behaviour at half-filling in magic-angle graphene superlattices

Yuan Cao, Valla Fatemi, Ahmet Demir, Shiang Fang, Spencer L. Tomarken, Jason Y. Luo, Javier D. Sanchez-Yamagishi, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, Ray C. Ashoori & Pablo Jarillo-Herrero

Nature **556**, 80–84(2018) | Cite this article



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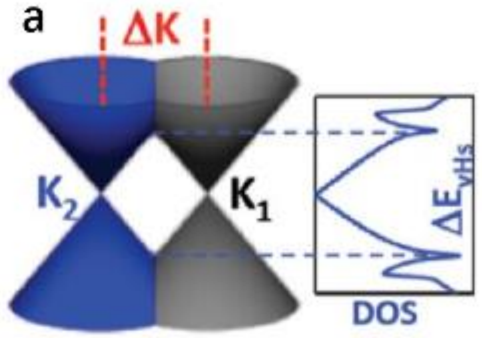
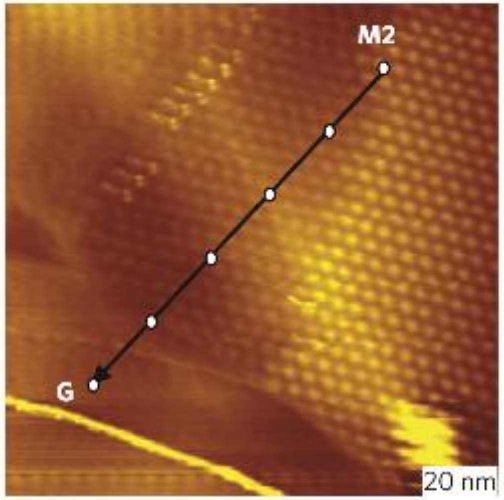
Van Hove singularity

The integrand of the density of states is divergent.

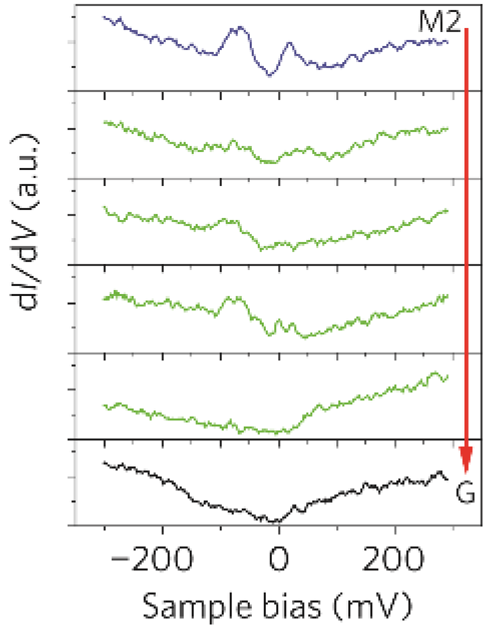


$$g(E) = \frac{L^3}{(2\pi)^3} \iint \frac{dk'_x \, dk'_y}{|\vec{\nabla} E|}$$

Topography near the boundary of the pattern



Spatial dependence of tunneling spectra along a line

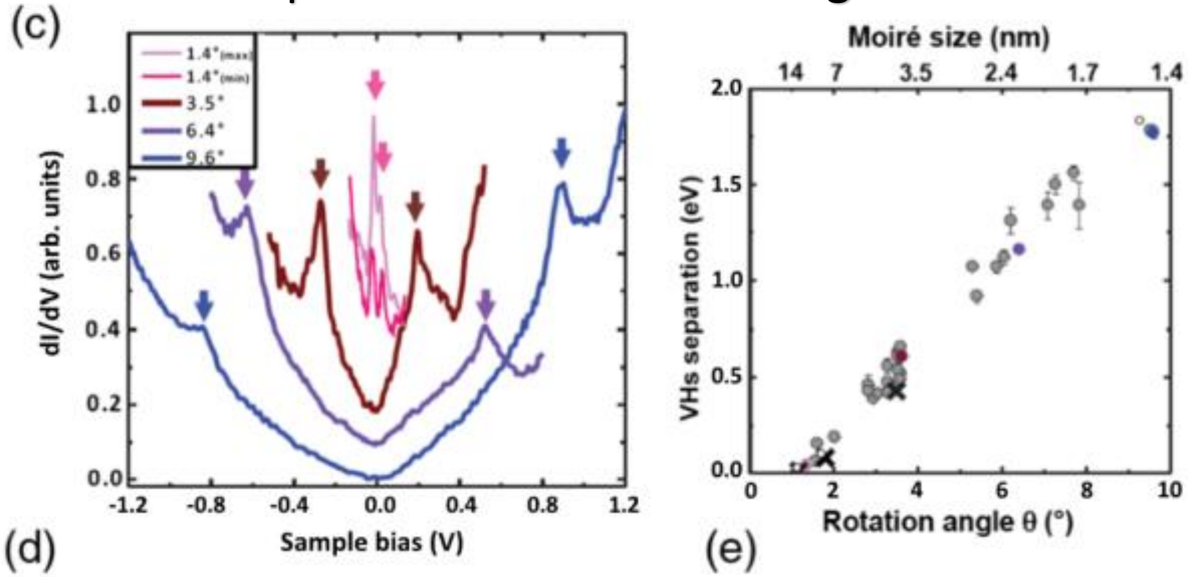


I. Brihuega et al, PRL 109, 196802 (2012)

Li, G.; Luican, A.; Lopes dos Santos, J.M.B.; Castro Neto, A.H.; Reina, A.; Kong, J.; Andrei, E.Y. Observation of Van Hove singularities in twisted graphene layers. Nat. Phys. 2010, 6, 109–113.

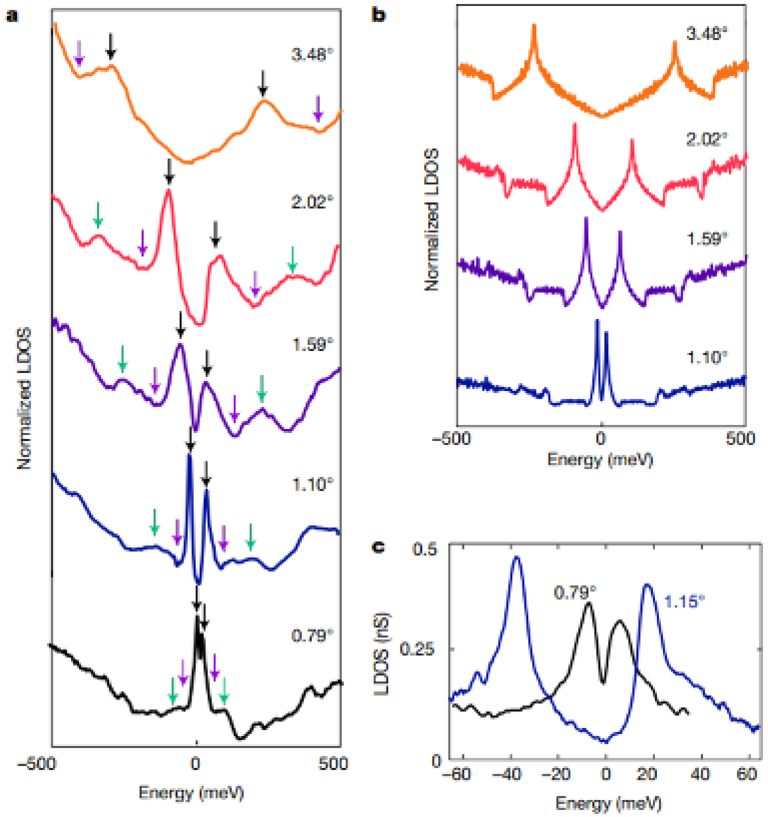
Van Hove singularity

The Van Hove singularity is in dependence of the twist angle.



$$\Delta E_{\mathrm{vHs}} = 2\hbar v_F \Gamma K \sin(\theta/2) - 2t_{\theta}$$

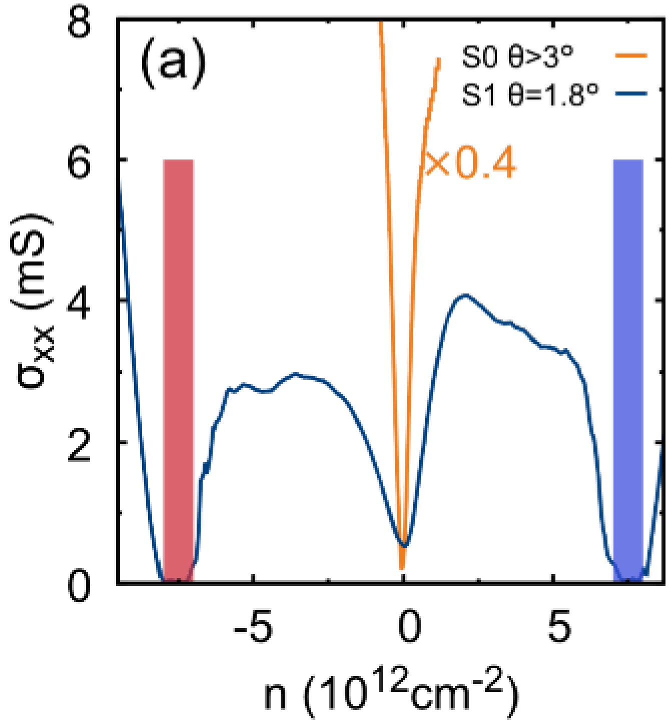
I. Brihuega et al, PRL 109, 196802 (2012)

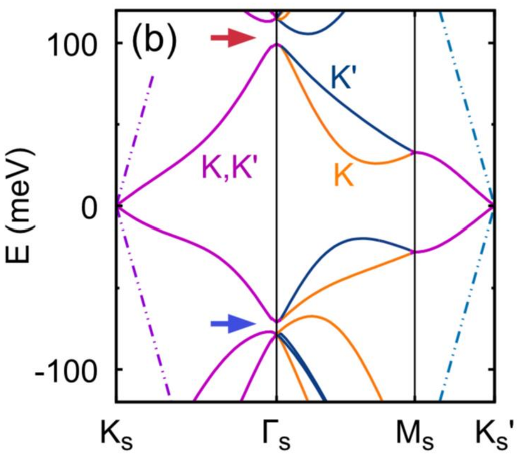


Choi, Y., Kemmer, J., Peng, Y. *et al.* Electronic correlations in twisted bilayer graphene near the magic angle. *Nat. Phys.* **15,** 1174–1180 (2019).

Mott insulator & Superconductivity

The conductance of different twist angles.



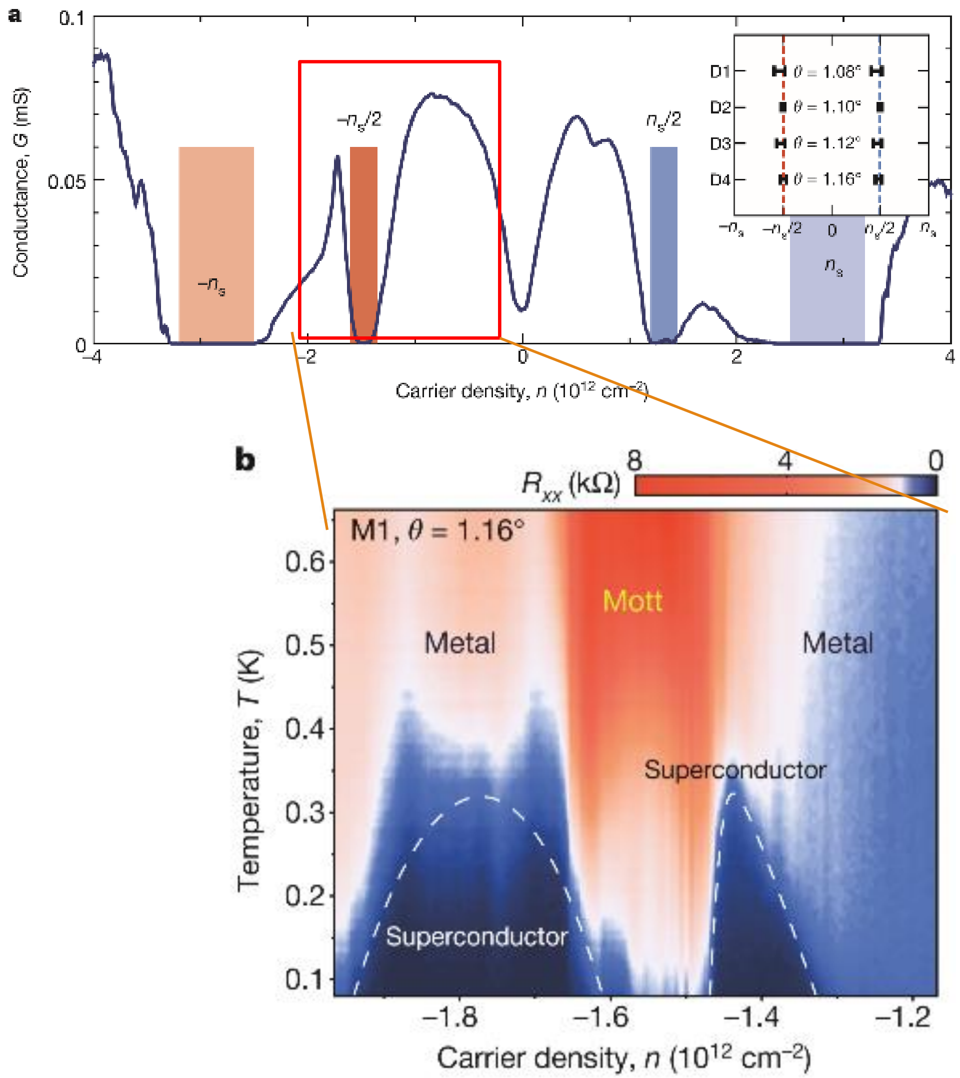


$n = 7.5 \times 10^{12}\ cm^{-2}$, is 4 times of the mini Brillouin zone area

$$A_{\mathrm{SL}} = 4/n = 53.3\ \mathrm{nm}^2 \qquad \Rightarrow \theta = 1.8^{\circ}$$

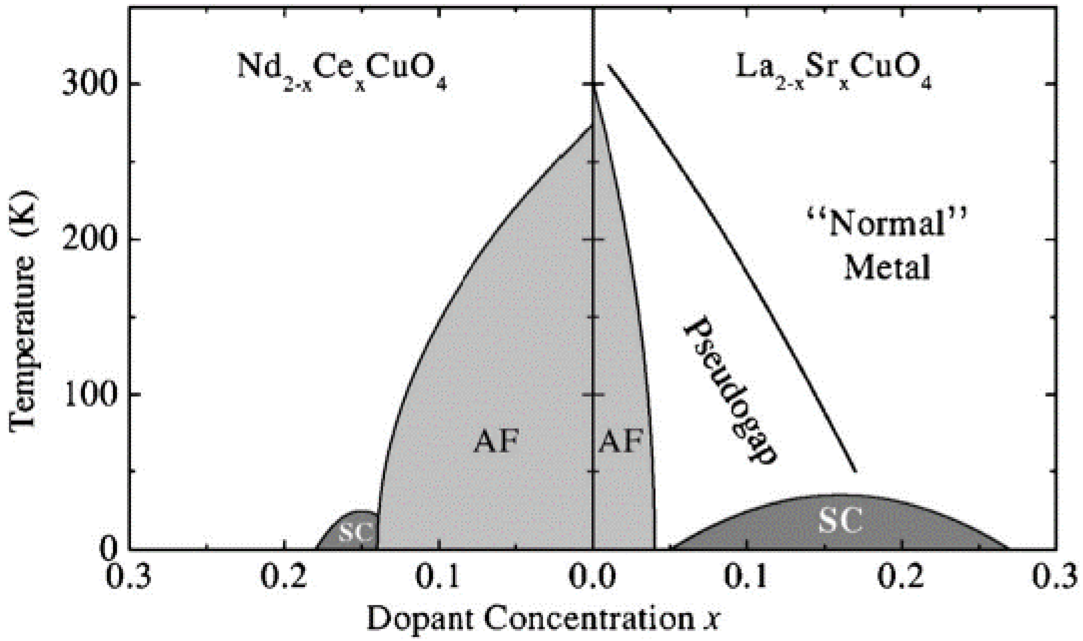
Cao, Y., Jarillo-Herrero, P. et al, Superlattice-Induced Insulating States and Valley-Protected Orbits in Twisted Bilayer Graphene. Phys. Rev. Lett. 2016, 117, 116804

Measured conductance G of magic-angle TBG device.



Mott insulator & Superconductivity

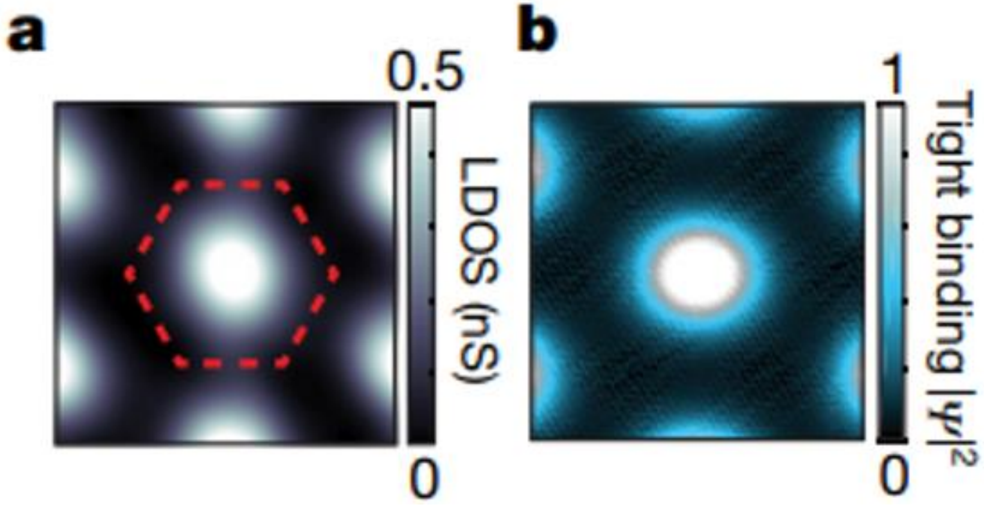
Schematic phase diagram of high-Tc superconductors showing hole doping right side and electron doping left side.



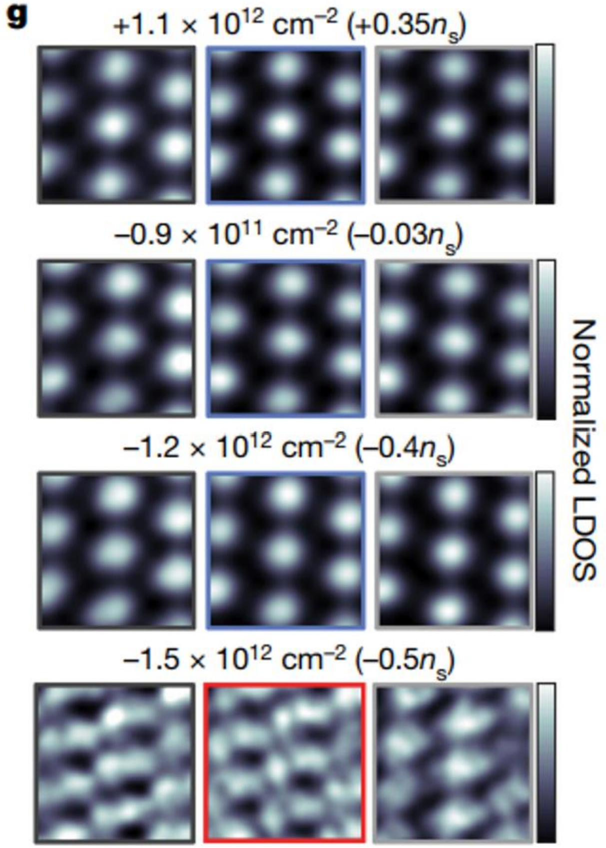
Cao, Y.; et al. Correlated insulator behaviour at half-filling in magic-angle graphene superlattices. Nature 2018, 556, 80–84

Cao, Y.; Jarillo-Herrero, P. ;et al, Unconventional superconductivity in magic-angle graphene superlattices. Nature 2018, 556, 43–50

Mott insulator & Superconductivity



C3-Symmetry breaking when the Fermi level attaches the half filling.

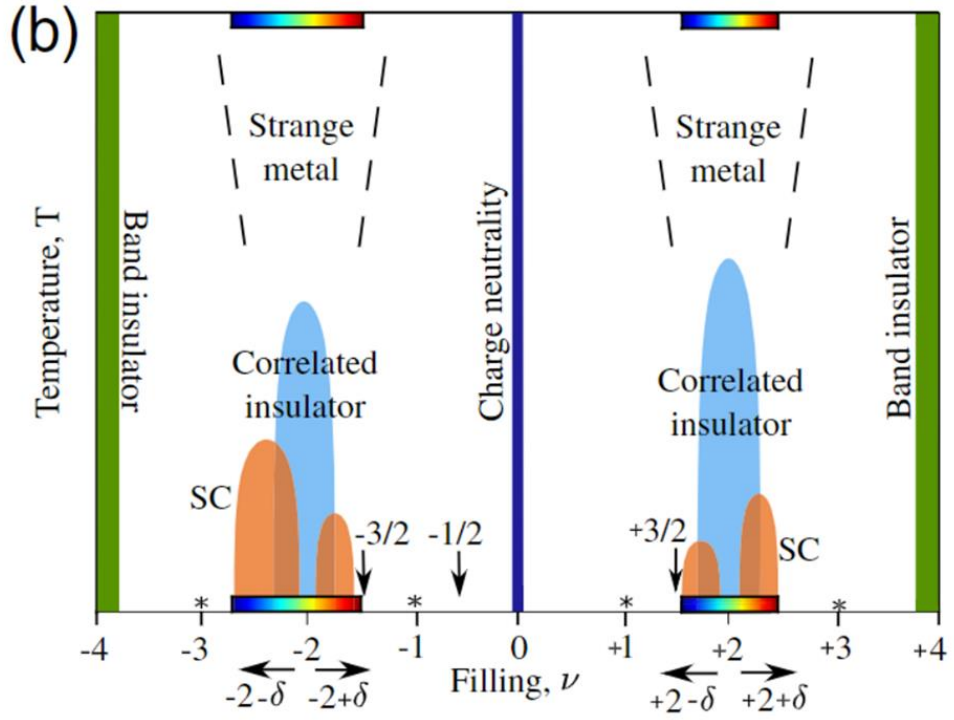


2019 Kerelsky, A. et al, Nature. Maximized electron interactions at the magic angle in twisted bilayer graphene

Summary

- Van Hove singularity
- Superconductor
- CDW
- Magnetism
- Strange metal
- …

- Twistronics
- Multilayer twistronics



2020 Cao, Y. et.al. PRL 124(7),076801

Thank you for attention