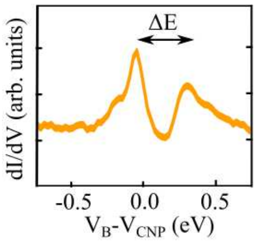
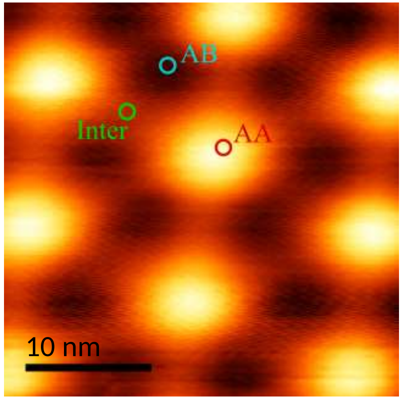
How heterostrain controls the flat bands of twisted bilayers of graphene ?

Scanning Tunneling Spectroscopy



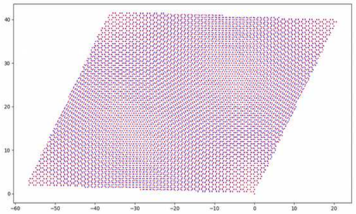
→ Information on the flat bands

Scanning Tunneling Microscopy



→ Information on heterostrain & stacking configuration

Link with Continuum and Tight binding calculations



The most important


Hartree-Fock
Continuum calculations
Tommaso Cea
Paco Guinea
IMDEA Nanosciencia

instituto imdea nanociencia


Tight binding calculations
Ahmed Missaoui
Guy Trambly de Laissardière
LPTM Cergy Pontoise

UNIVERSITÉ de Cergy-Pontoise

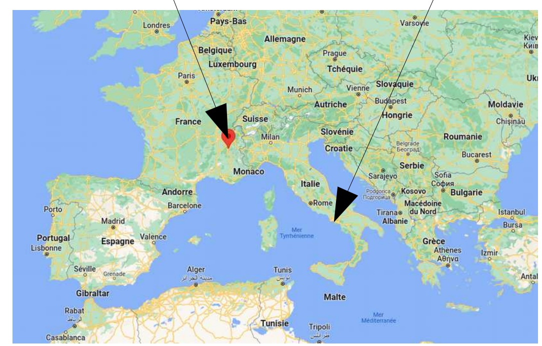


STM team
Loic Huder
Vincent T. Renard
Claude Chapelier
IRIG PHELIQS

cea

UNIVERSITÉ Grenoble Alpes

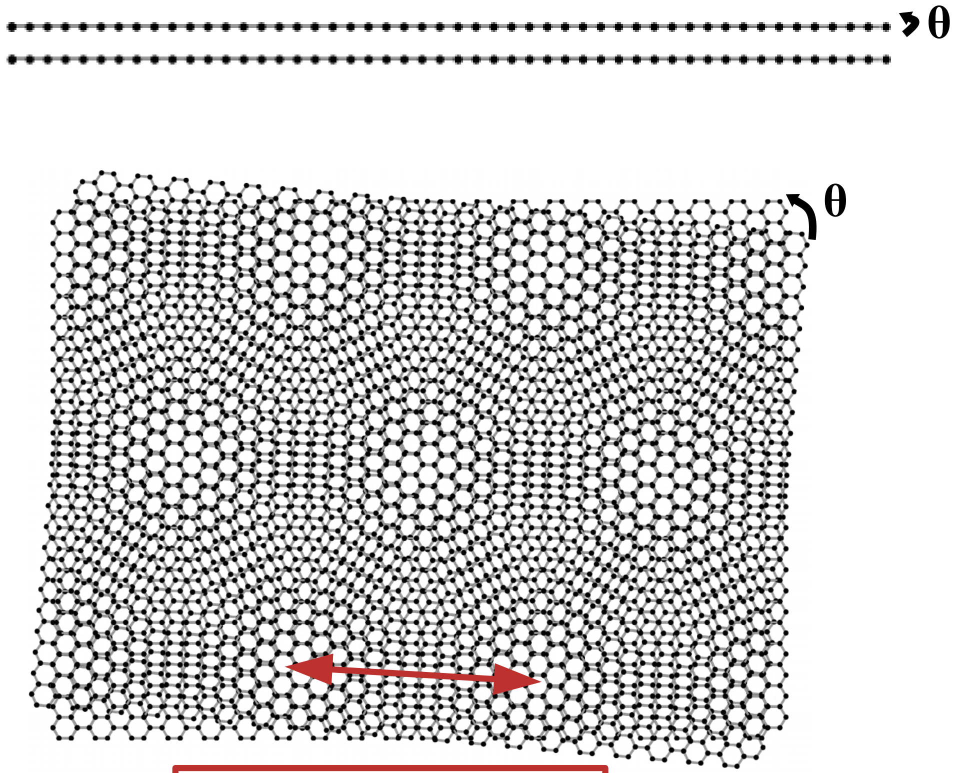
Capri Spring School



Reference: F. Mesple* *et al.* Phys. Rev. Lett. 127, 126405, 2021

*florie.mesple@cea.fr

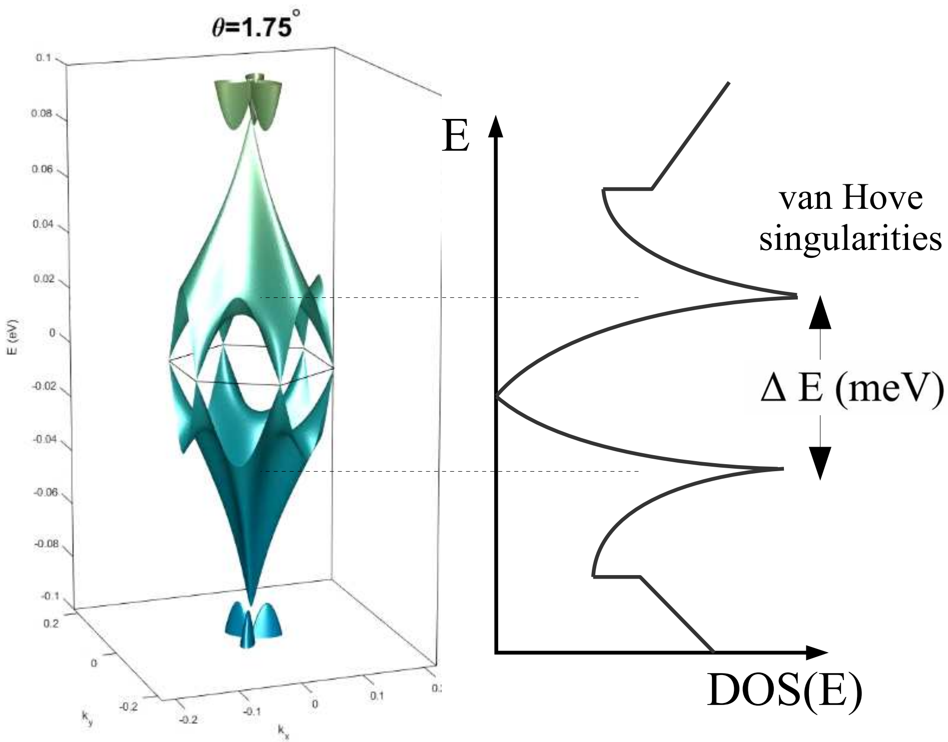
Twisting two layers of graphene



$$a_M = \frac{a_{Gr}}{2sin(\theta/2)}$$

Flat-bands in low angle twisted bilayers of graphene

Highly tunable system



Y. Cao et al. Nature 556, 80 (2019)

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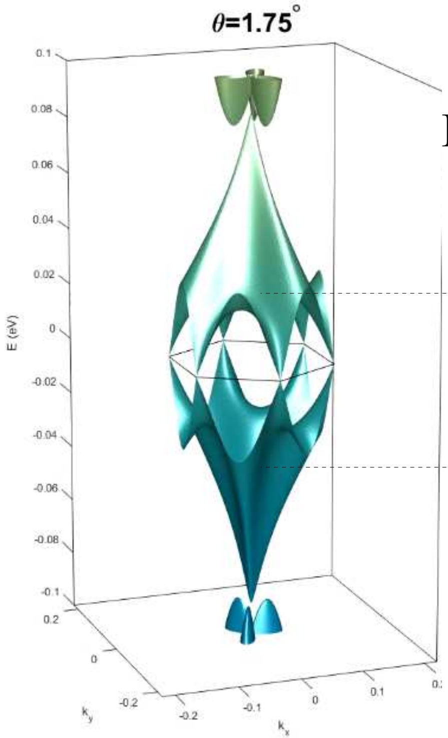

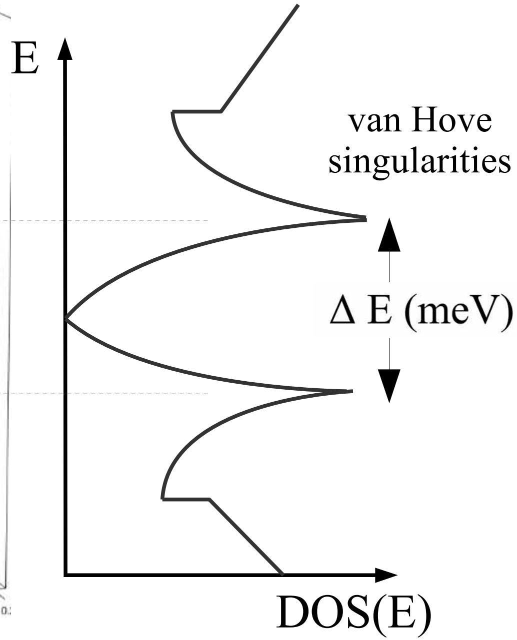

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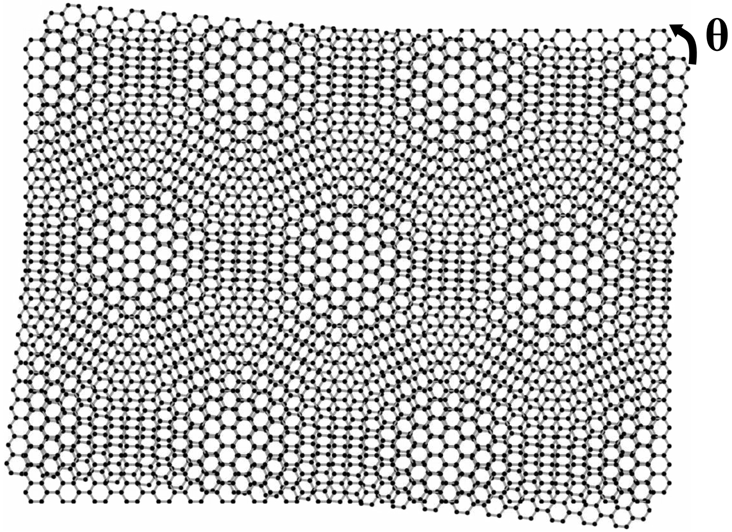

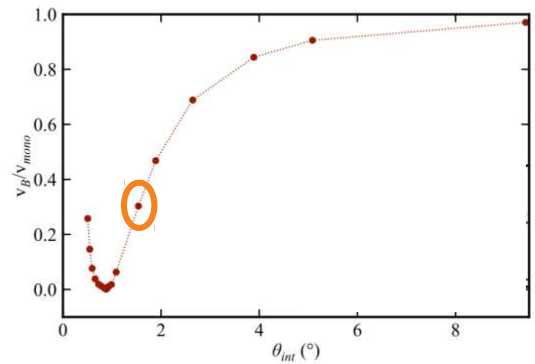

G. T. de Laissardière et. al ; Nano Lett. 10, 804-808 (2010)

R. Bistritzer and A. H. MacDonald. PNAS 108(30), (2011)

J. M. B. Lopes dos Santos et al P.R.B 86, 155449, (2012)

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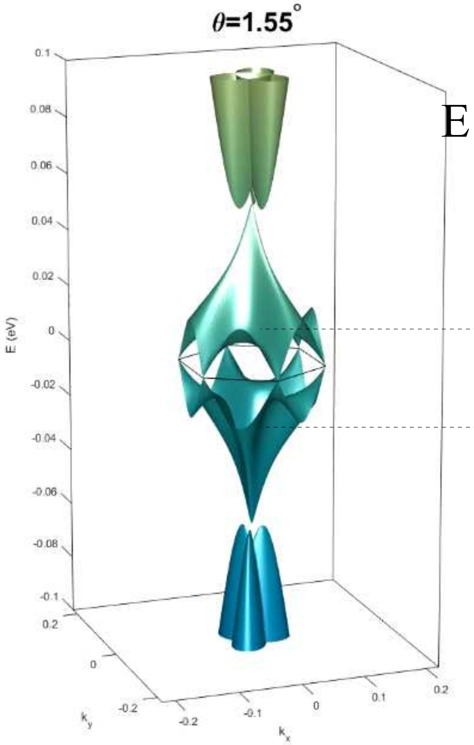
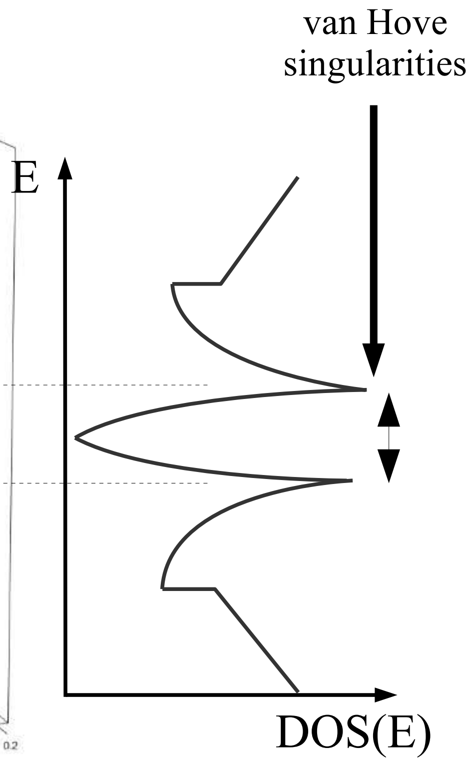
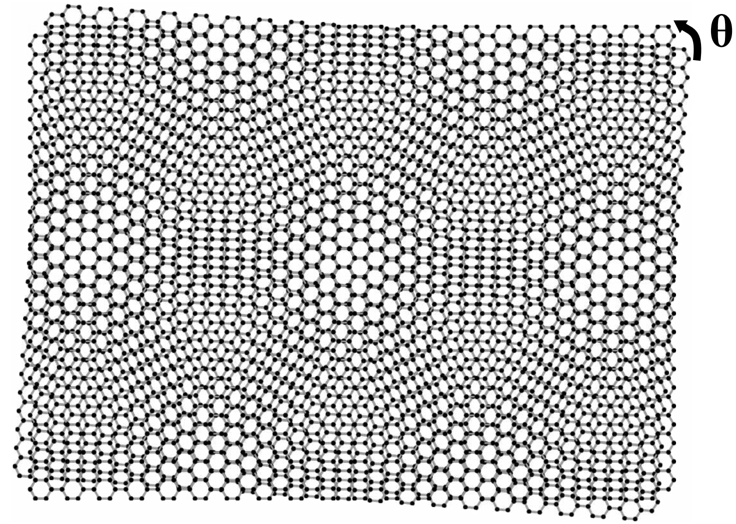
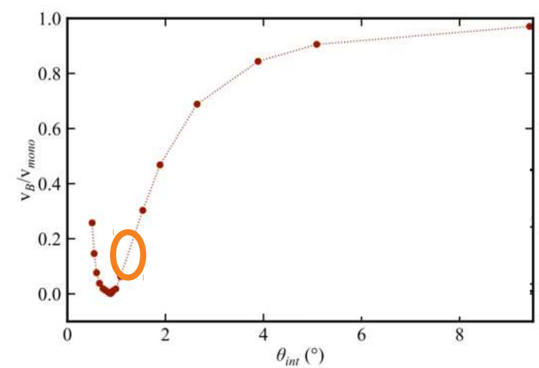




Y. Cao et al. Nature 556, 80 (2019)





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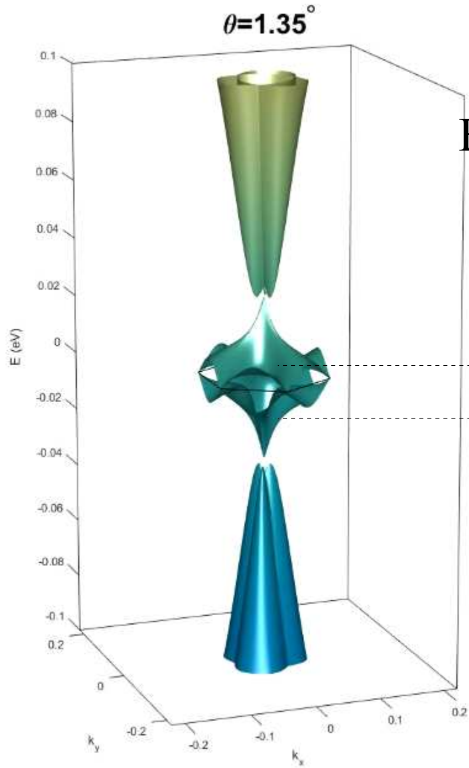
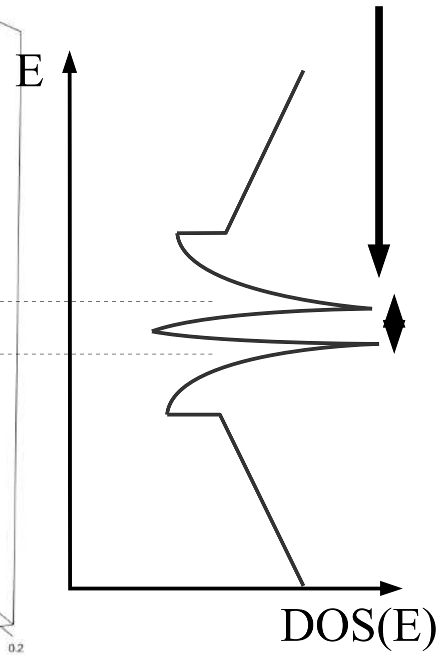
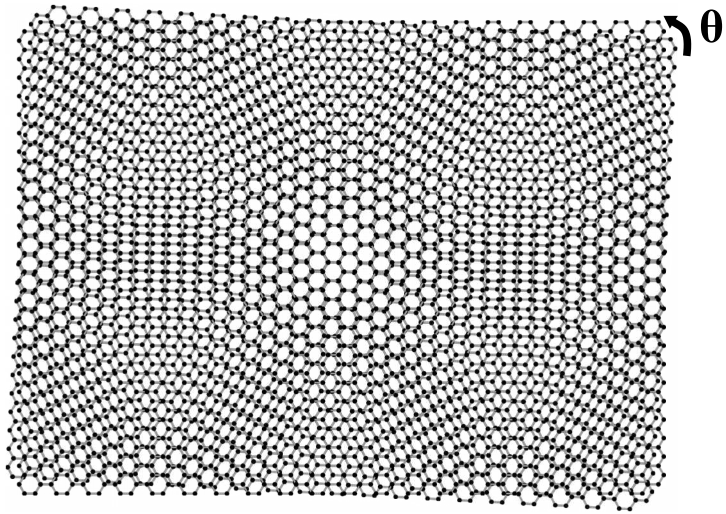
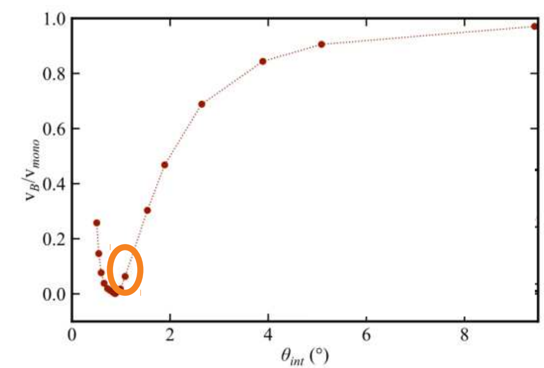




Y. Cao et al. Nature 556, 80 (2019)





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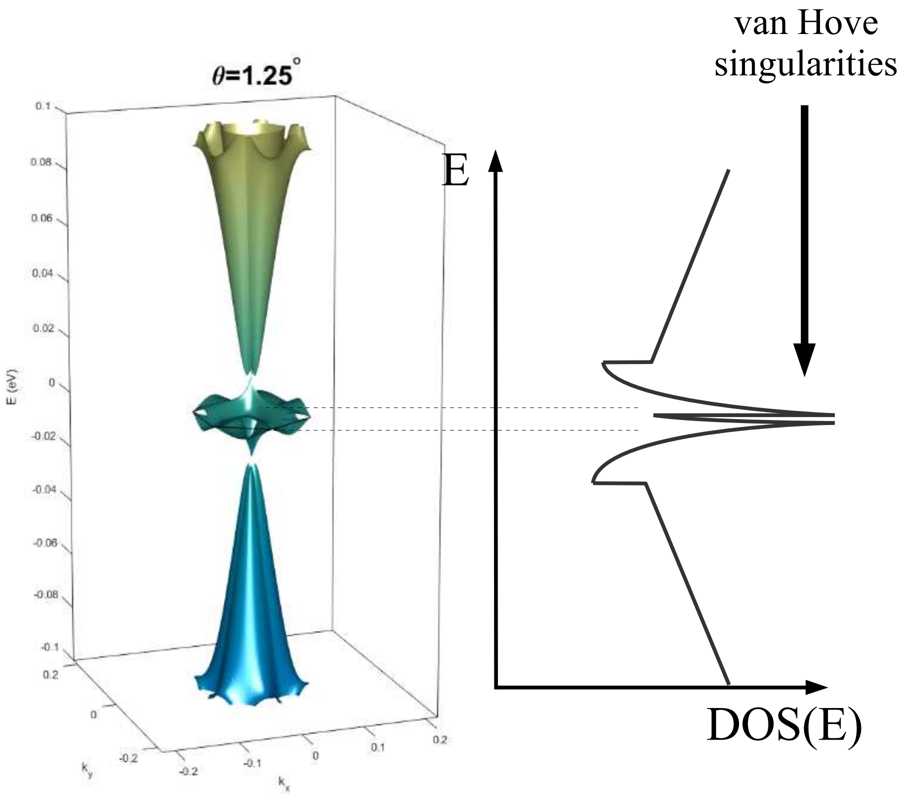

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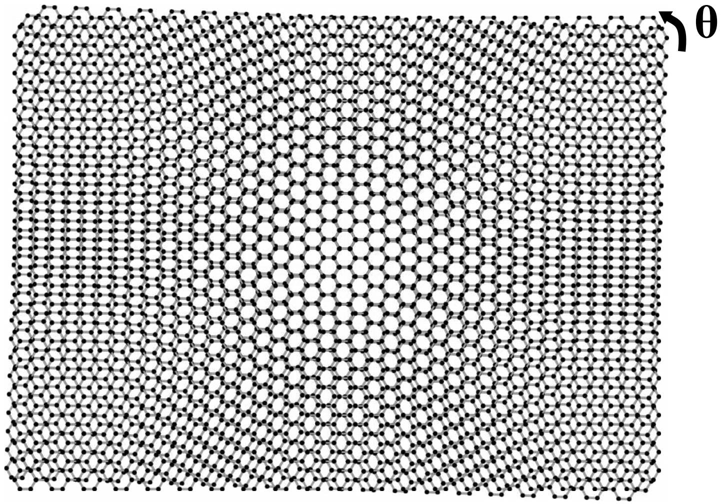

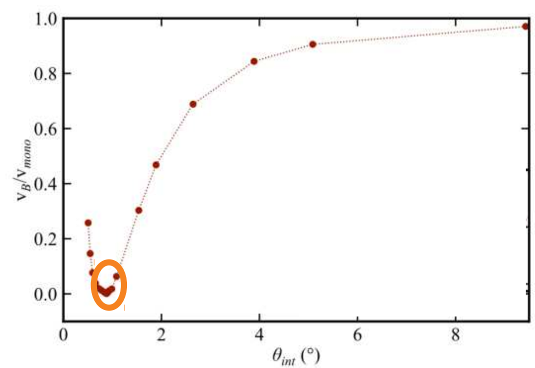

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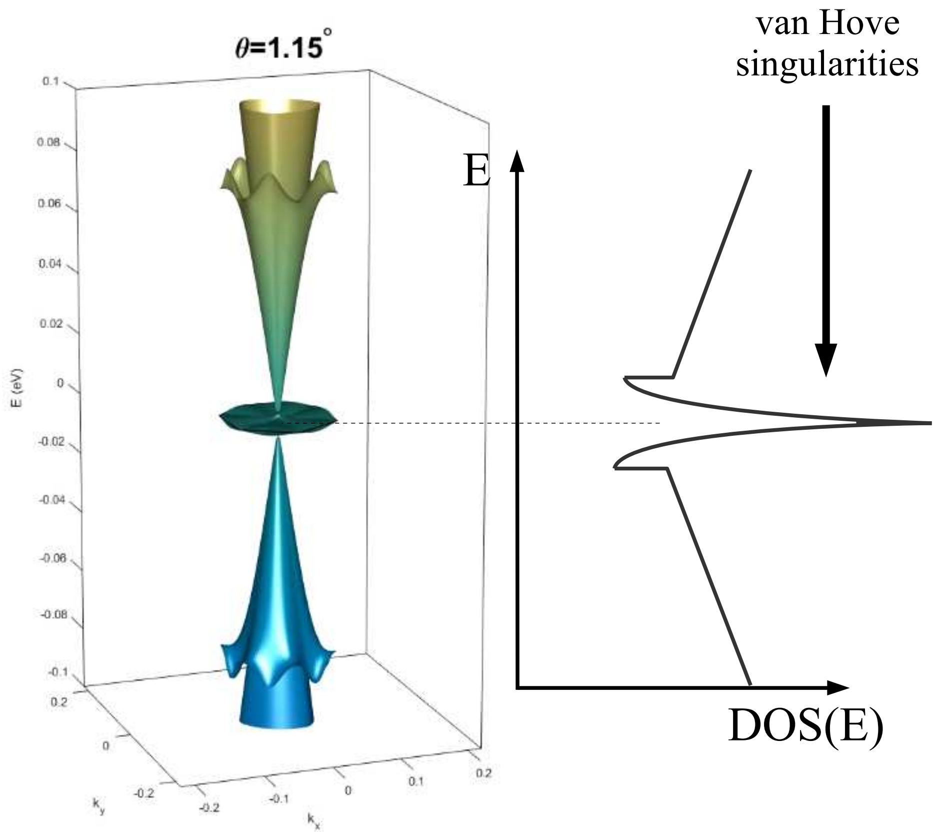

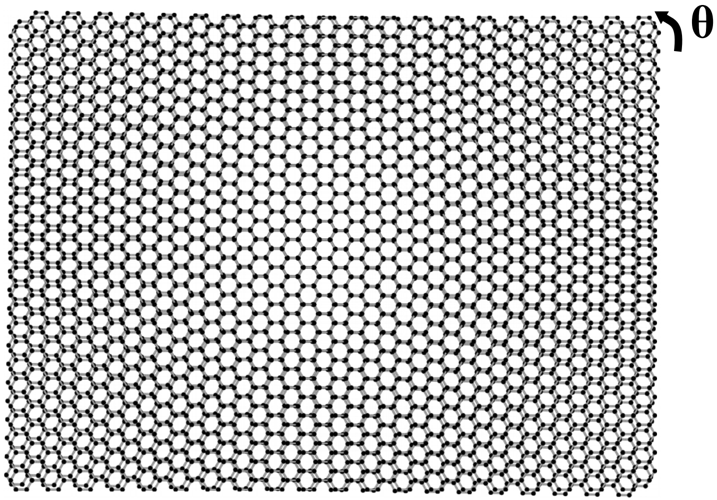

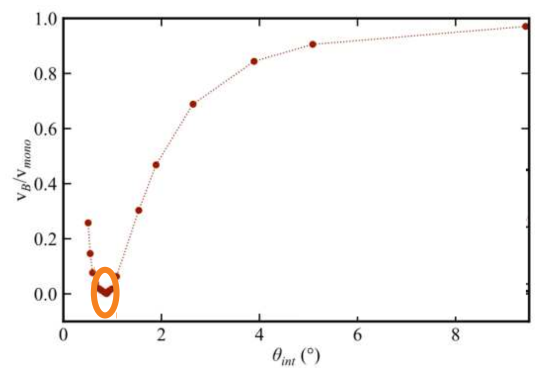

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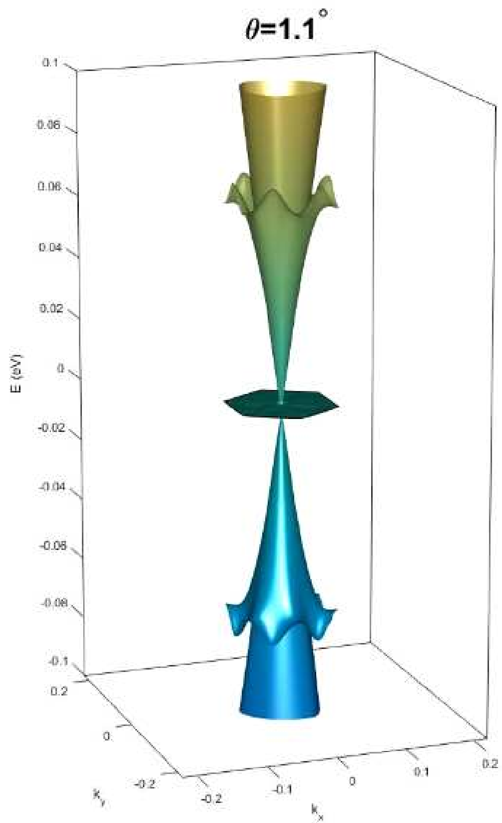
Highly tunable system

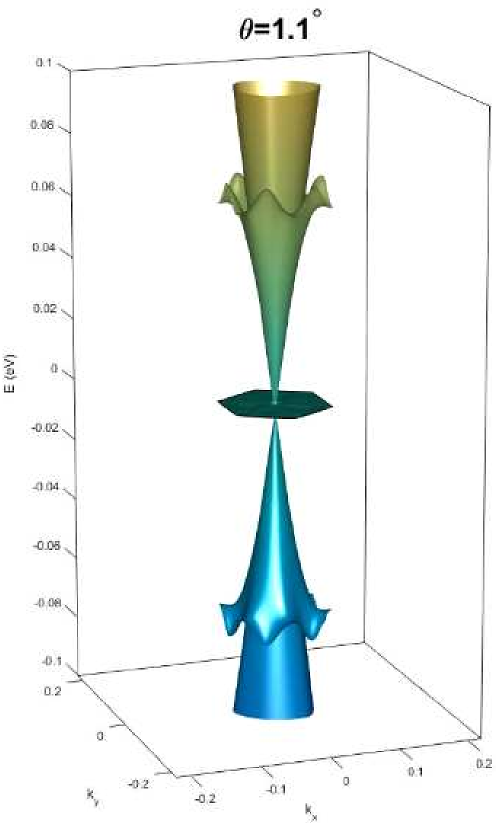


Y. Cao et al. Nature 556, 80 (2019)

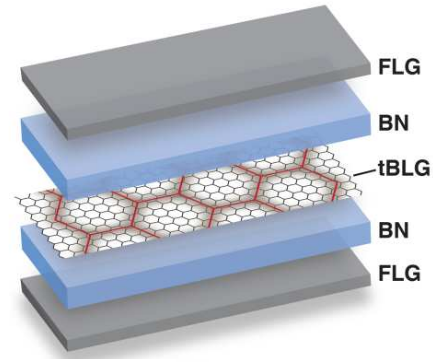
$$\frac{E_C}{E_k} \to \infty$$ ⟹ boosted interactions

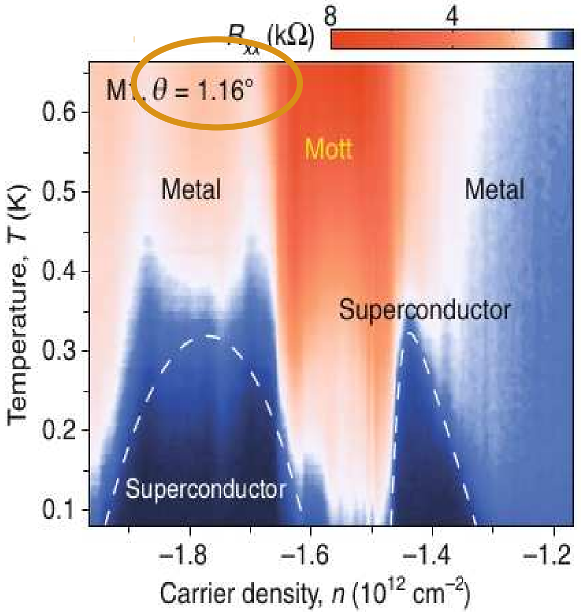
Measurement of correlated states

Highly tunable system



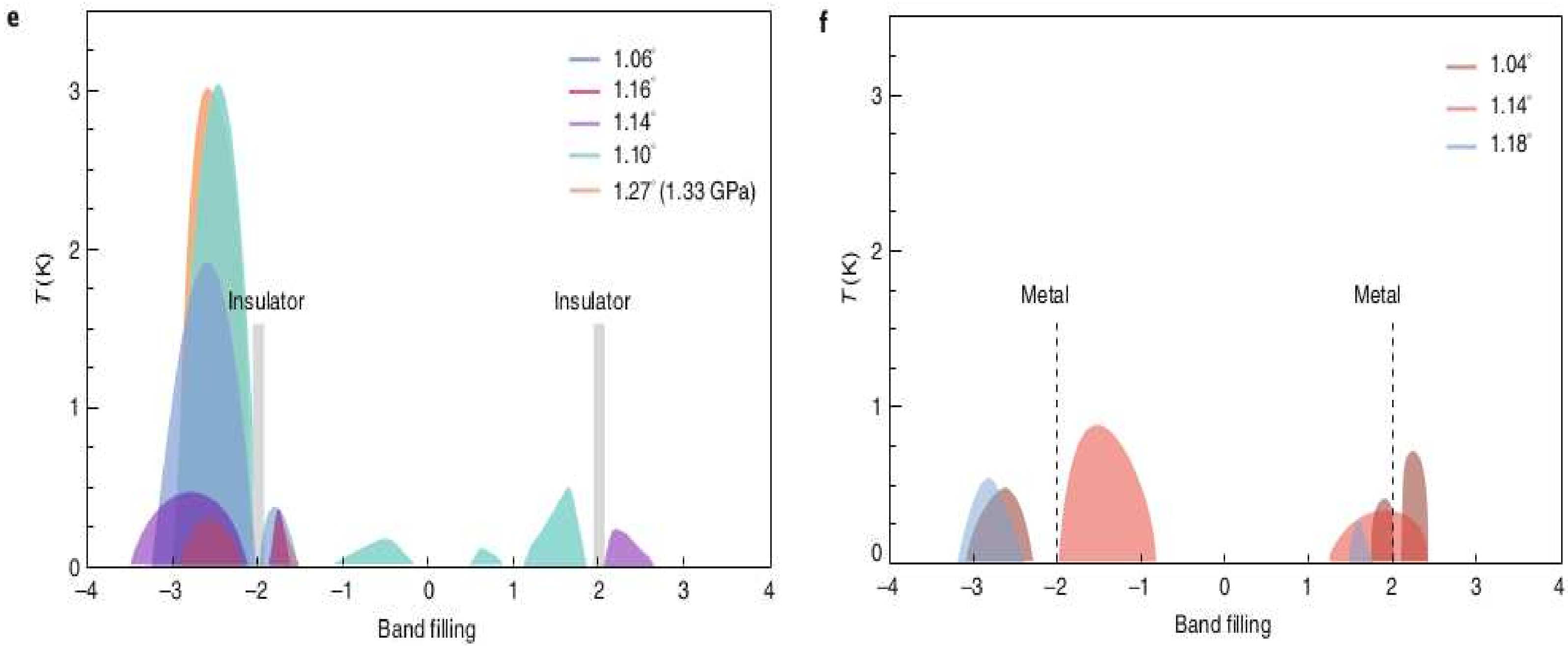
Y. Cao et al. Nature 556, 80 (2019)



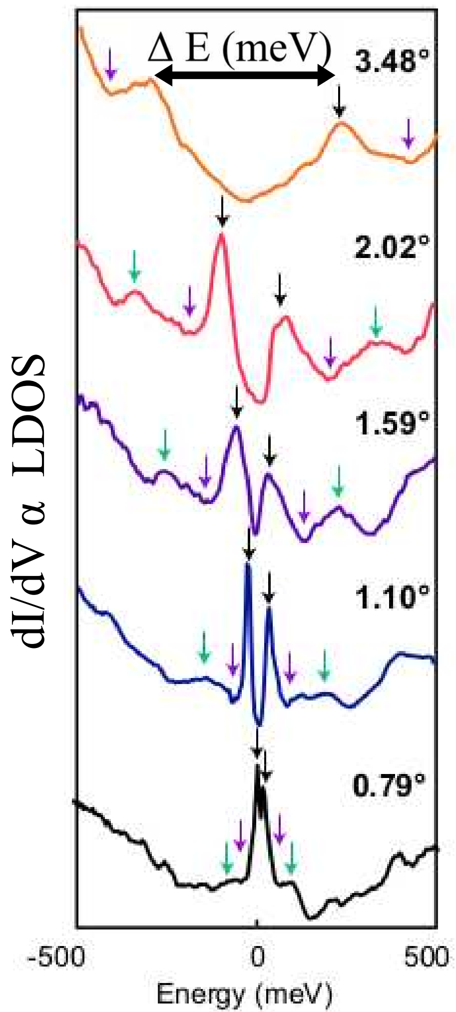


Y. Cao et al. Nature 55, 43-50, (2019)

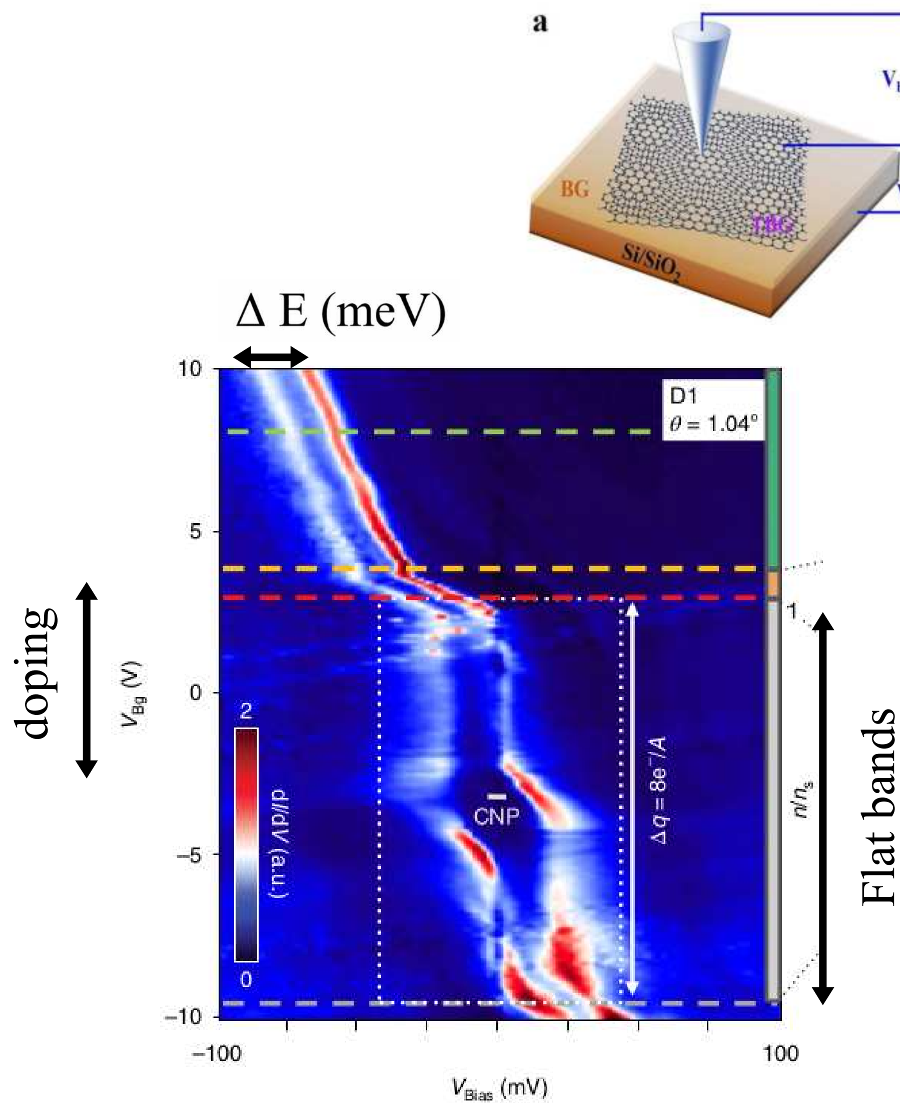
L. Balents, C. R. Dean, D. K. Efetov, and A. F. Young Nature Physics 16(7), 725-733 (2020)



Tracking the vHs with STS

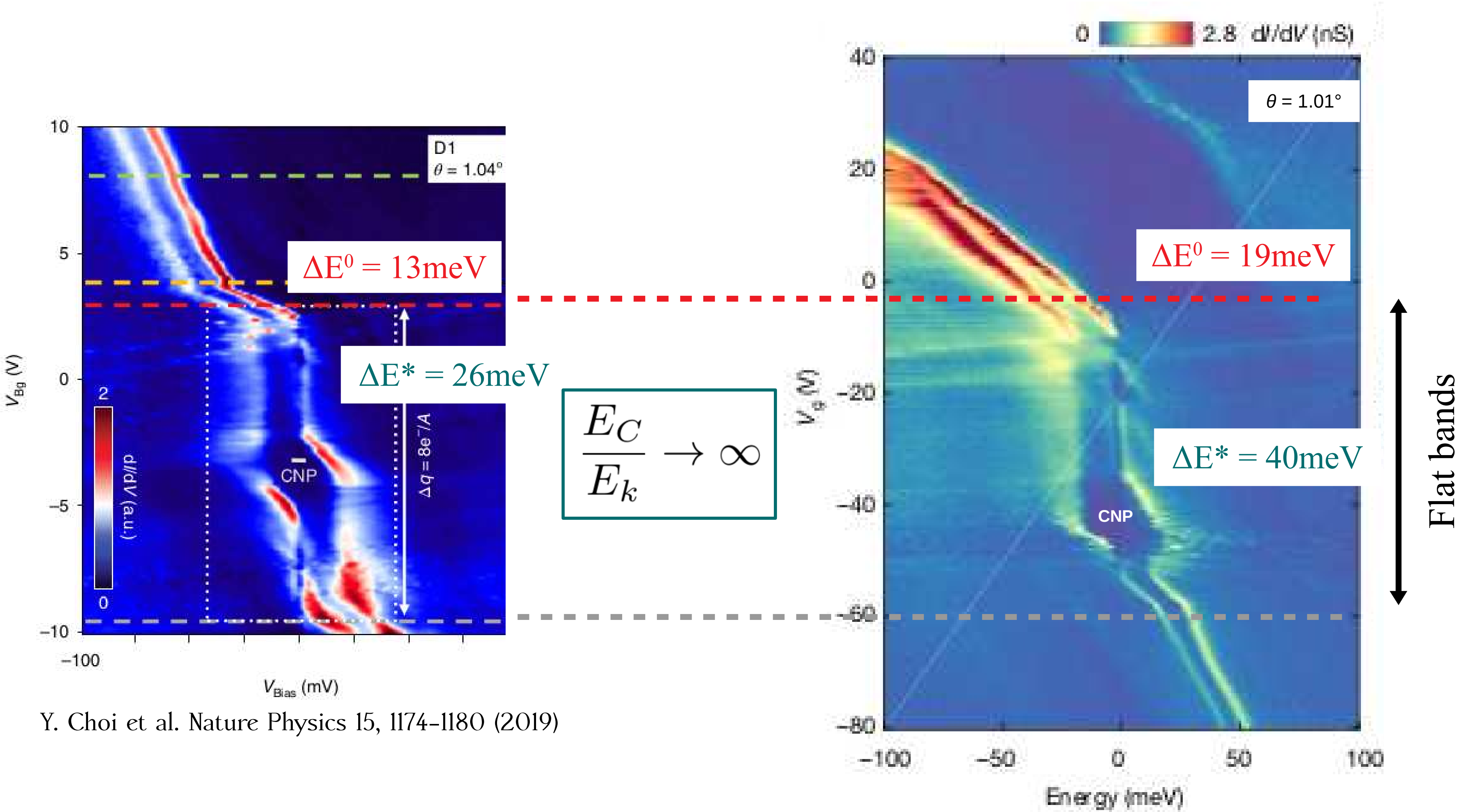


A. Kerelsky et al. Nature 572, 95-100 (2019)



Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

A variety of Twisted bilayers of graphene



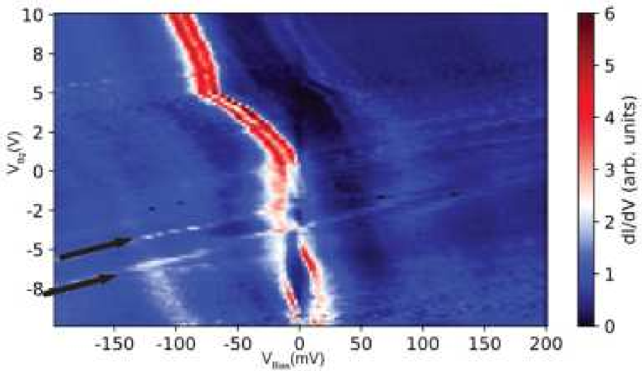
$$\frac{E_C}{E_k} \to \infty$$

Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

Y. Xie et al. Nature 572, 101-105 (2019)

A variety of Twisted bilayers of graphene

3.



1. L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)
2. A. Kerelsky et al. Nature 572, 95-100 (2019)
3. Y. Choi et al. Nature Physics 15, 1174-1180 (2019)
4. Y. Jiang et al. Nature 573, 91-95 (2019)
5. Y. Xie et al. Nature 572, 101-105 (2019)
6. Z. Zhang et al. Phys. Rev. Research 2, 033181 (2020)
7. D. Wong et al. Nature 582(7811), 198-202 (2020)
8. Y. Choi et al. arXiv 2008.11746 (2020)
9. K. P. Nuckolls et al. arXiv 2007.03810 (2020)

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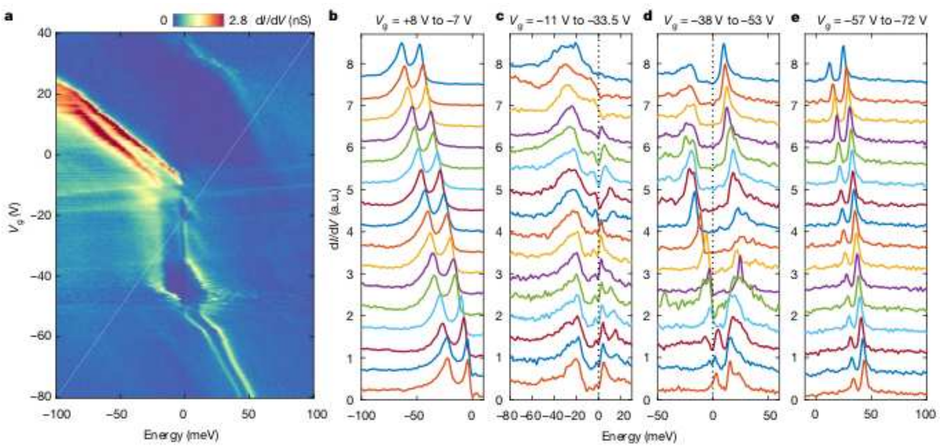

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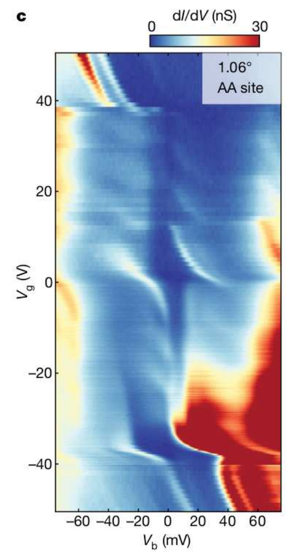

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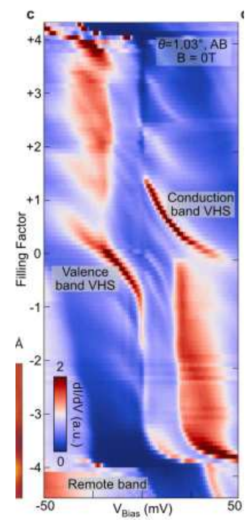

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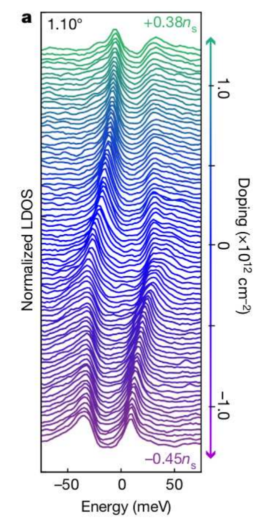
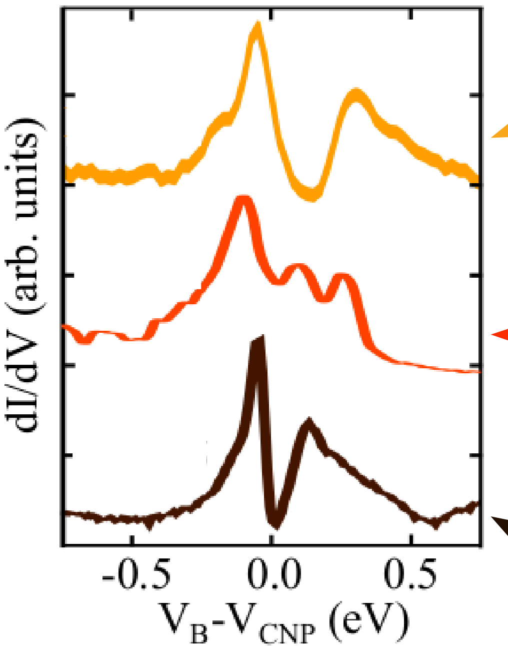
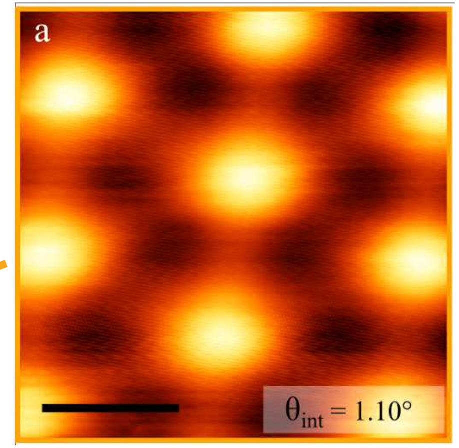


A sensitive system





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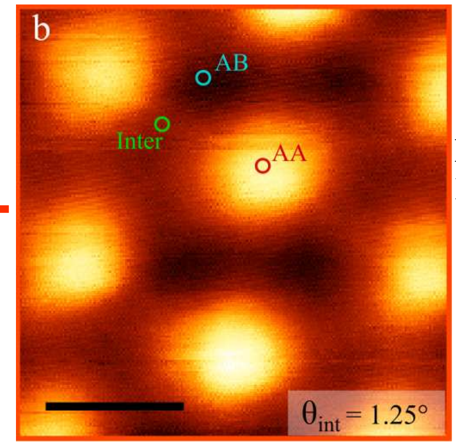

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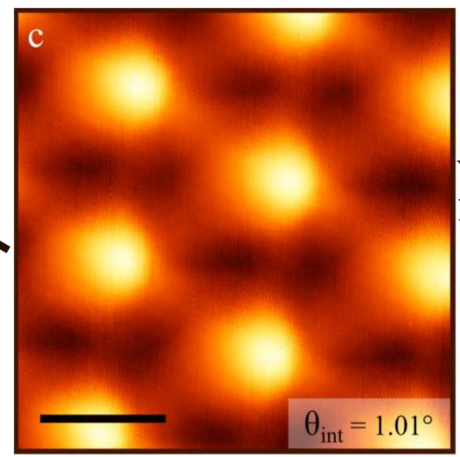
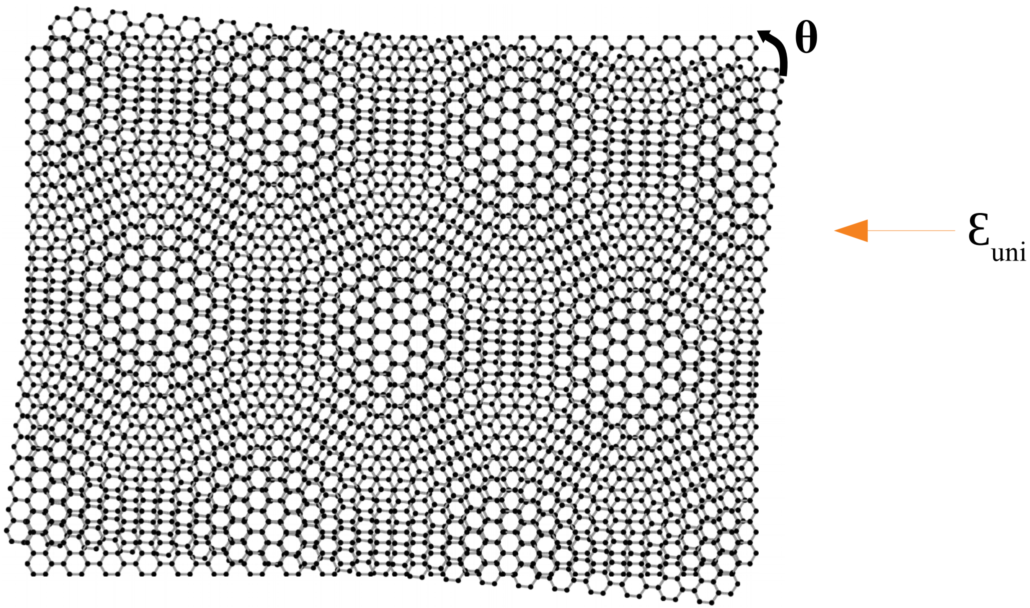


Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

Heterostrain : schematic view

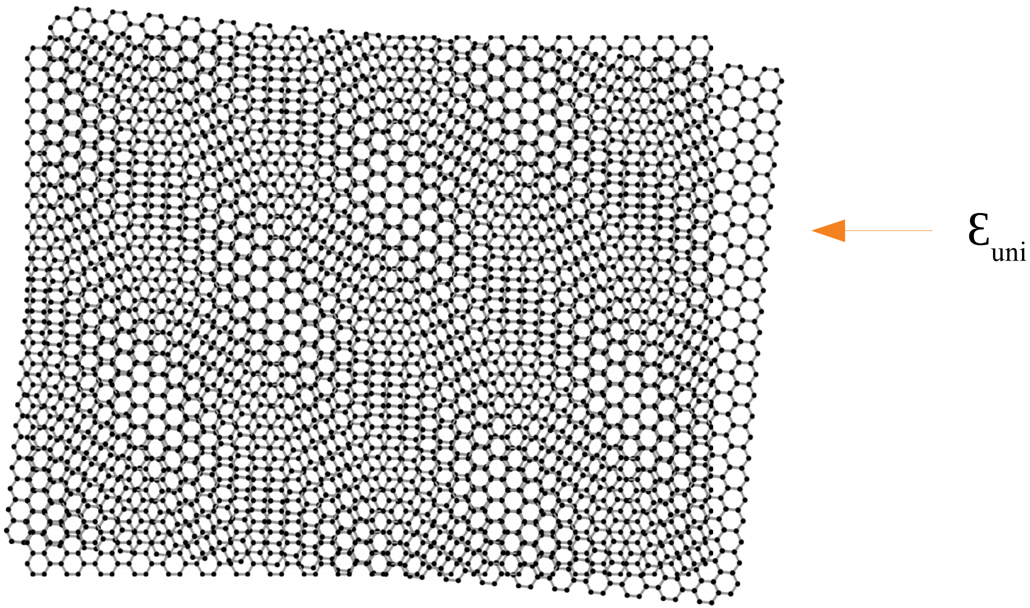
- θ
- ε_{uni}



$$\begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix}$$

Heterostrain : schematic view

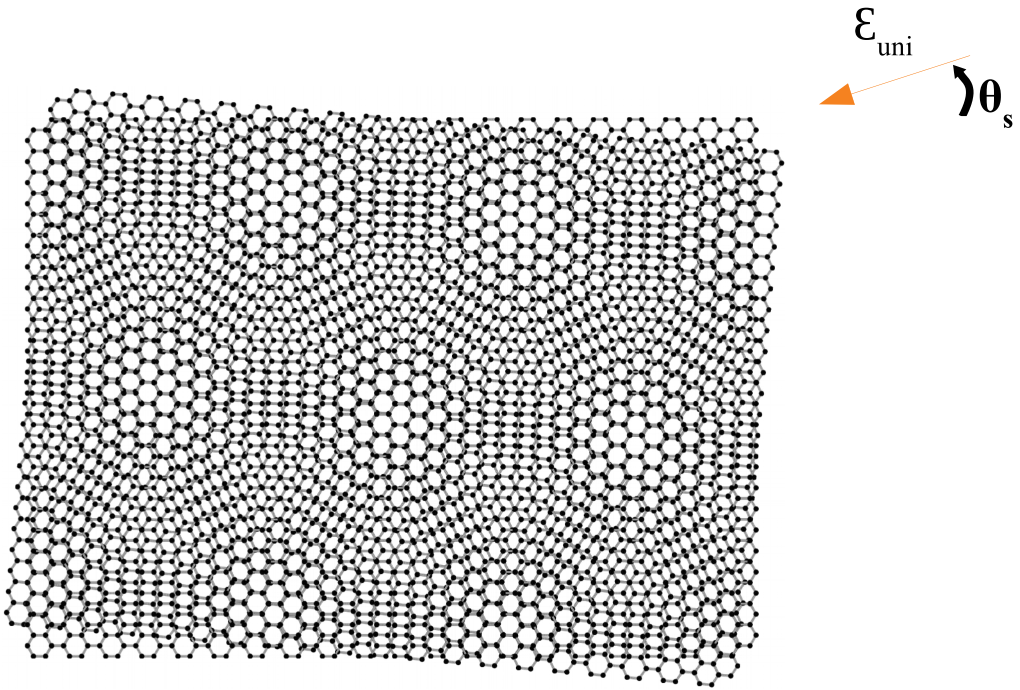
- **θ**
- ε_{uni}



$$\begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix}$$

Heterostrain : schematic view

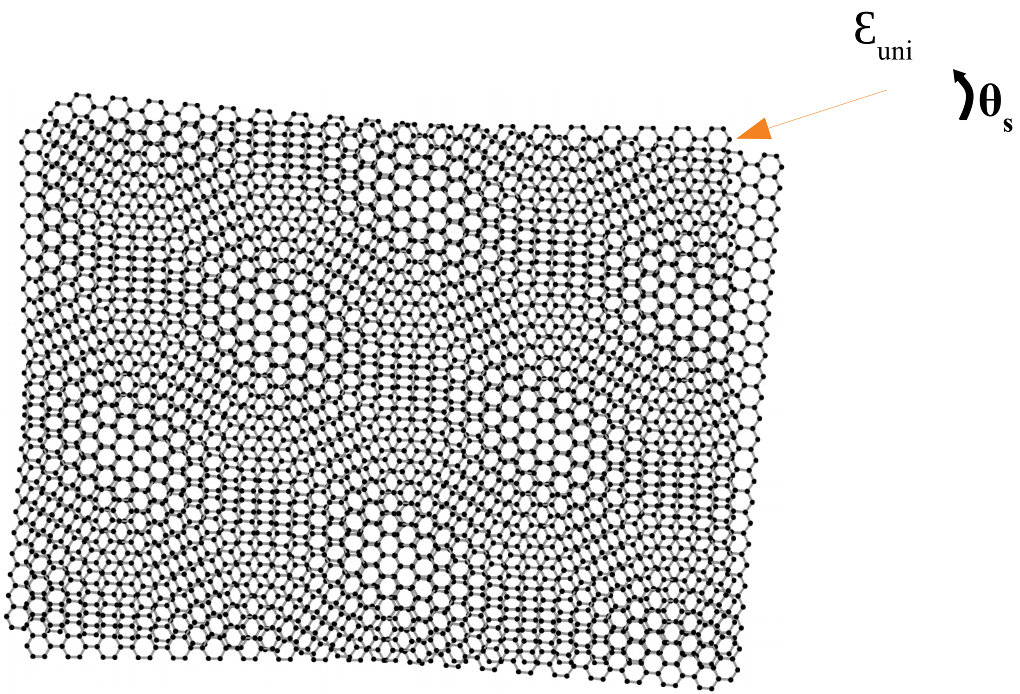
- θ
- ε_{uni}
- θ_s



$$\begin{pmatrix} cos\theta_2 & -sin\theta_2 \\ sin\theta_2 & cos\theta_2 \end{pmatrix} \begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} cos\theta_1 & -sin\theta_1 \\ sin\theta_1 & cos\theta_1 \end{pmatrix}$$

Heterostrain : schematic view

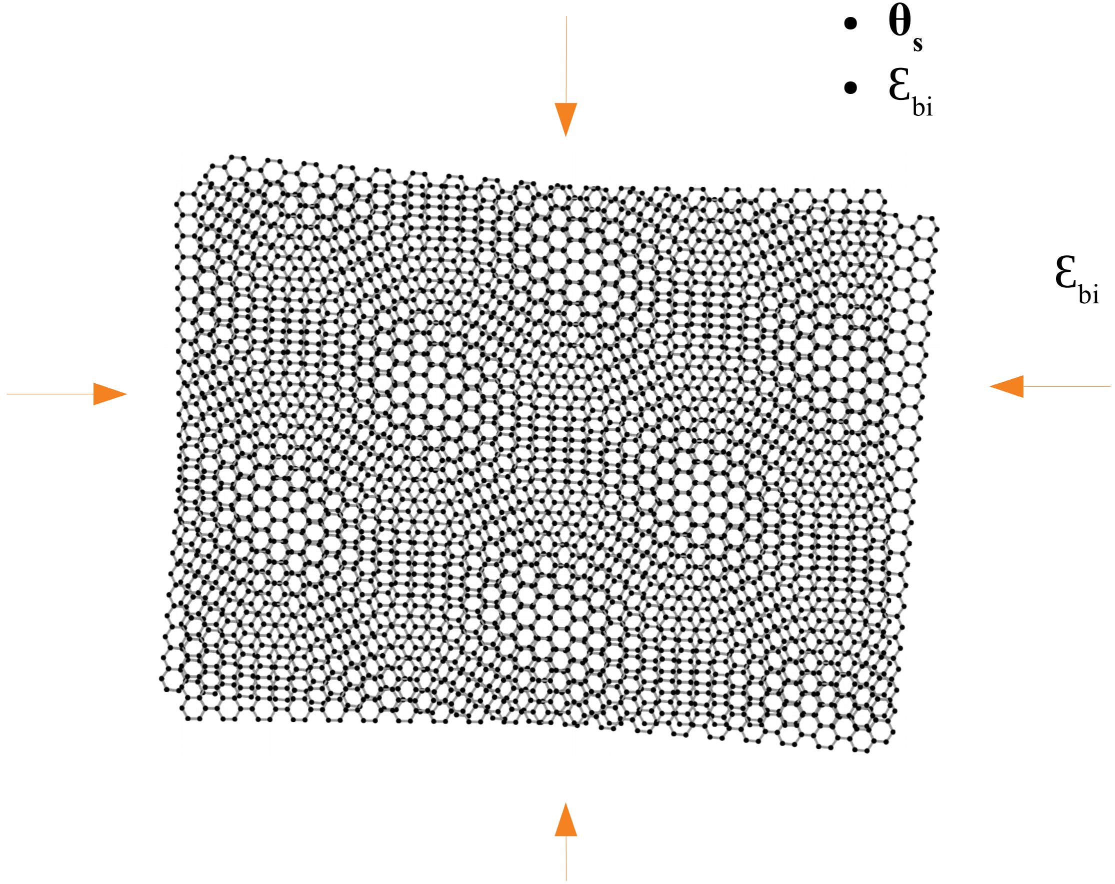
- **θ**
- ε_{uni}
- θ_s



$$\begin{pmatrix} cos\theta_2 & -sin\theta_2 \\ sin\theta_2 & cos\theta_2 \end{pmatrix} \begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} cos\theta_1 & -sin\theta_1 \\ sin\theta_1 & cos\theta_1 \end{pmatrix}$$

Heterostrain : schematic view

- θ
- ε_{uni}
- θ_s
- ε_{bi}

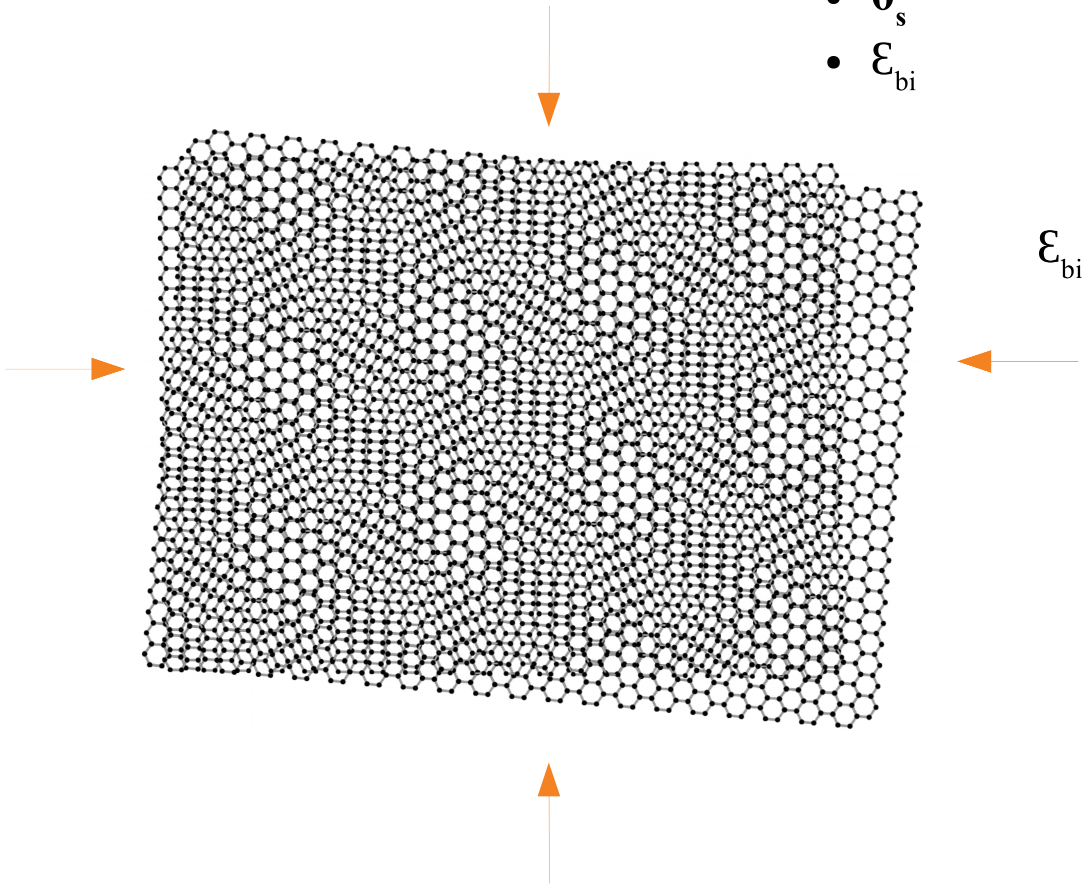


$$\begin{pmatrix} cos\theta_2 & -sin\theta_2 \\ sin\theta_2 & cos\theta_2 \end{pmatrix} \begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} cos\theta_1 & -sin\theta_1 \\ sin\theta_1 & cos\theta_1 \end{pmatrix} \begin{pmatrix} (\varepsilon_{bi}+1) & 0 \\ 0 & (\varepsilon_{bi}+1) \end{pmatrix}$$

Heterostrain : schematic view

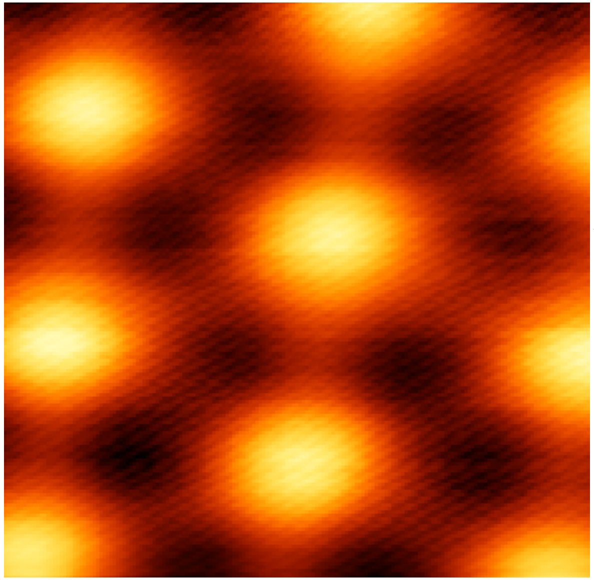
- **θ**
- ε_{uni}
- θ_s
- ε_{bi}

A. Artaud et al. Scientific Reports 6, 25670 (2016)

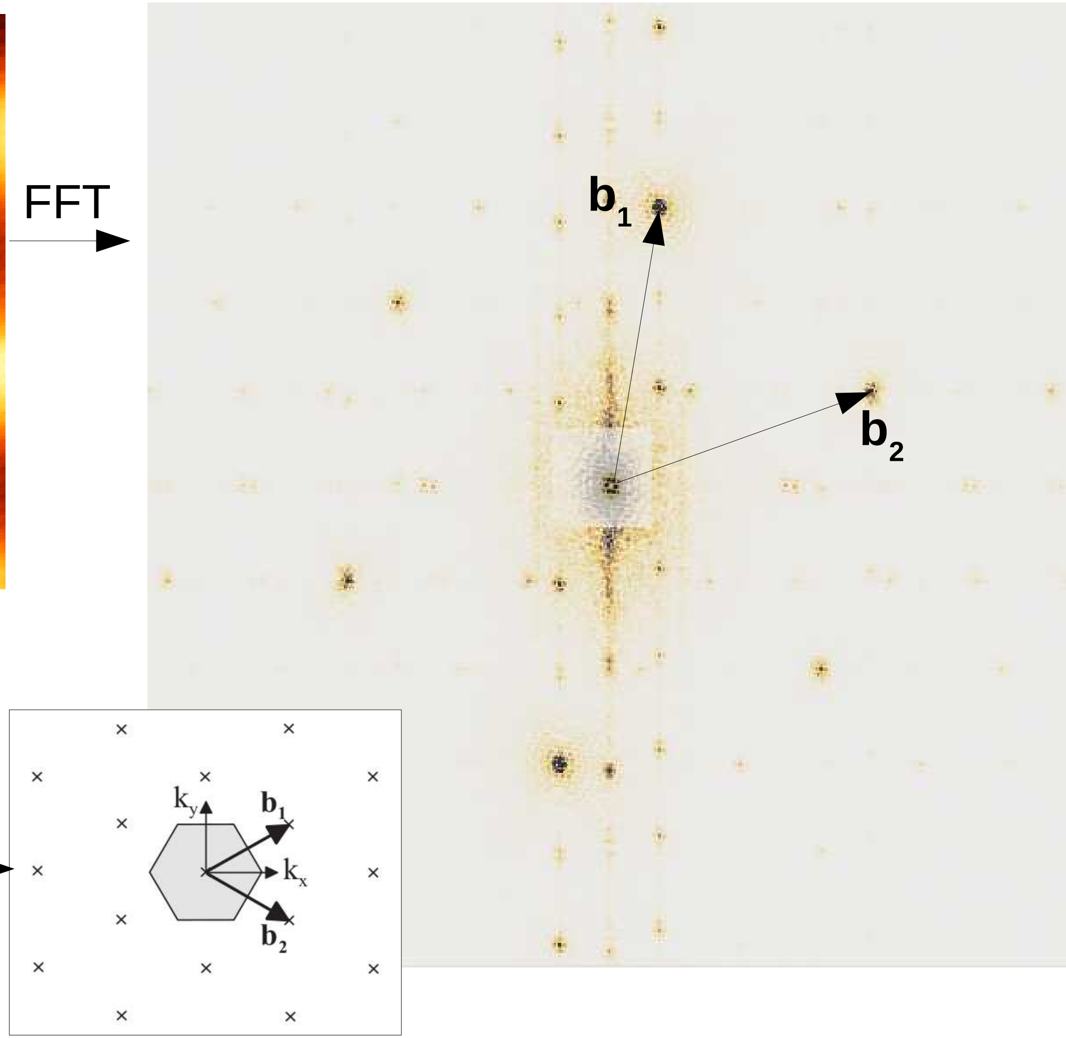


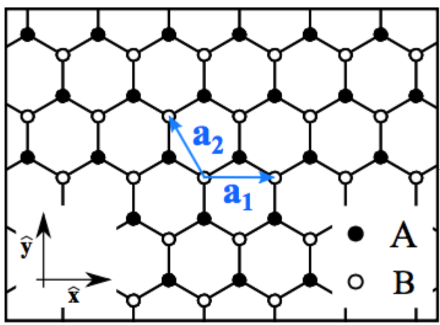
$$\begin{pmatrix} a_{t_1} \\ a_{t_2} \end{pmatrix} = \begin{pmatrix} cos\theta_2 & -sin\theta_2 \\ sin\theta_2 & cos\theta_2 \end{pmatrix} \begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} cos\theta_1 & -sin\theta_1 \\ sin\theta_1 & cos\theta_1 \end{pmatrix} \begin{pmatrix} (\varepsilon_{bi}+1) & 0 \\ 0 & (\varepsilon_{bi}+1) \end{pmatrix} \begin{pmatrix} a_{b_1} \\ a_{b_2} \end{pmatrix}$$

Heterostrain in experiments



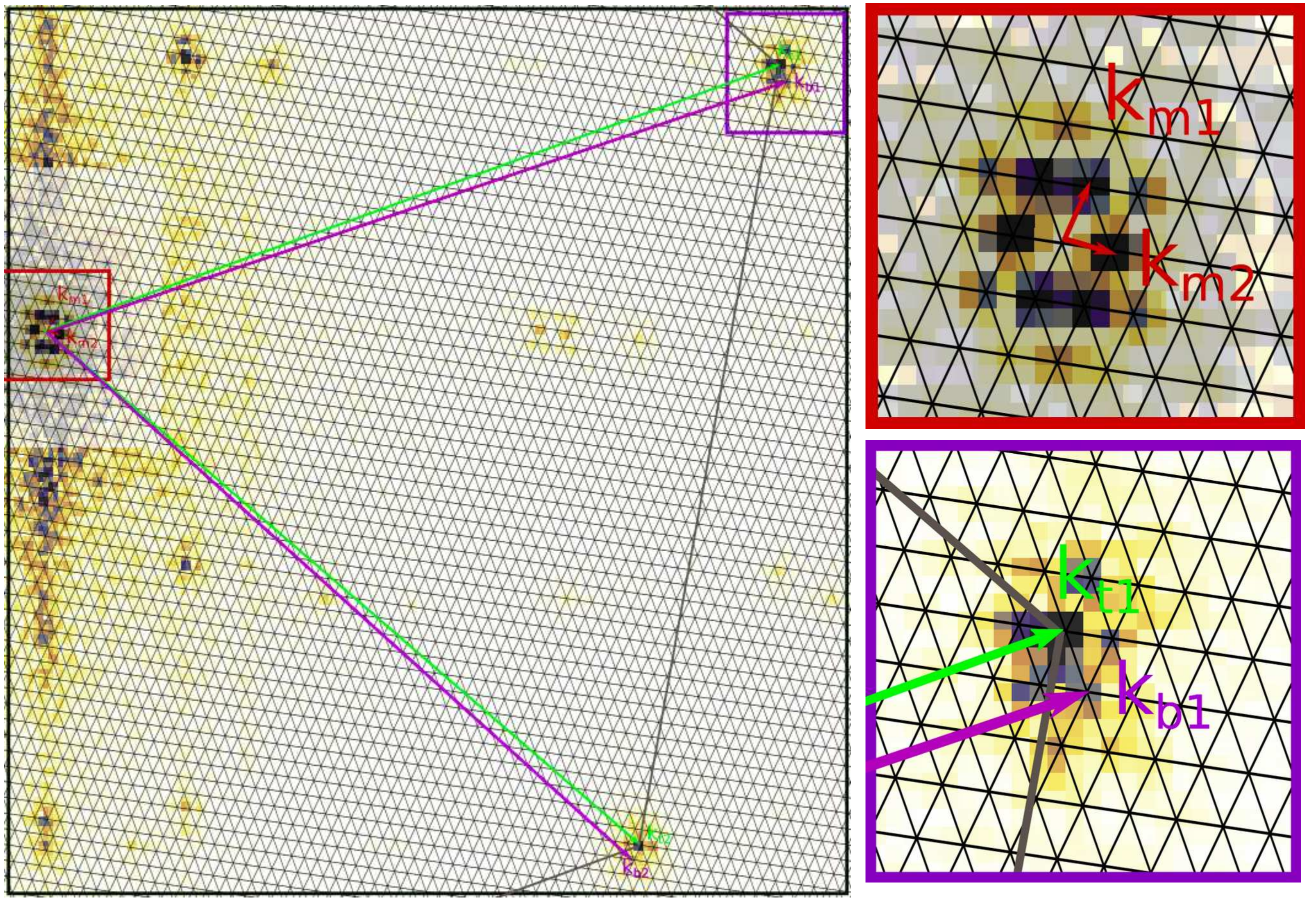
FFT





FT

Heterostrain in experiments



$$\begin{pmatrix} k_{b_1} \\ k_{b_2} \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} k_{t_1} \\ k_{t_2} \end{pmatrix}$$

↓

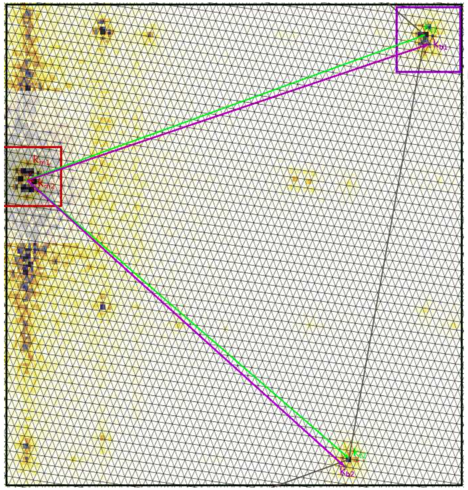
No calibration artefacts

Commensurate cell :

$$\begin{pmatrix} k_{t_1} \\ k_{t_2} \end{pmatrix} = \begin{pmatrix} i & k \\ j & l \end{pmatrix} \begin{pmatrix} k_{m_1} \\ k_{m_2} \end{pmatrix} = \begin{pmatrix} 29 & 34 \\ -23 & 66 \end{pmatrix} \begin{pmatrix} k_{m_1} \\ k_{m_2} \end{pmatrix}$$

$$\begin{pmatrix} k_{b_1} \\ k_{b_2} \end{pmatrix} = \begin{pmatrix} m & q \\ n & r \end{pmatrix} \begin{pmatrix} k_{m_1} \\ k_{m_2} \end{pmatrix} = \begin{pmatrix} 28 & 35 \\ -24 & 66 \end{pmatrix} \begin{pmatrix} k_{m_1} \\ k_{m_2} \end{pmatrix}$$

Heterostrain in experiments



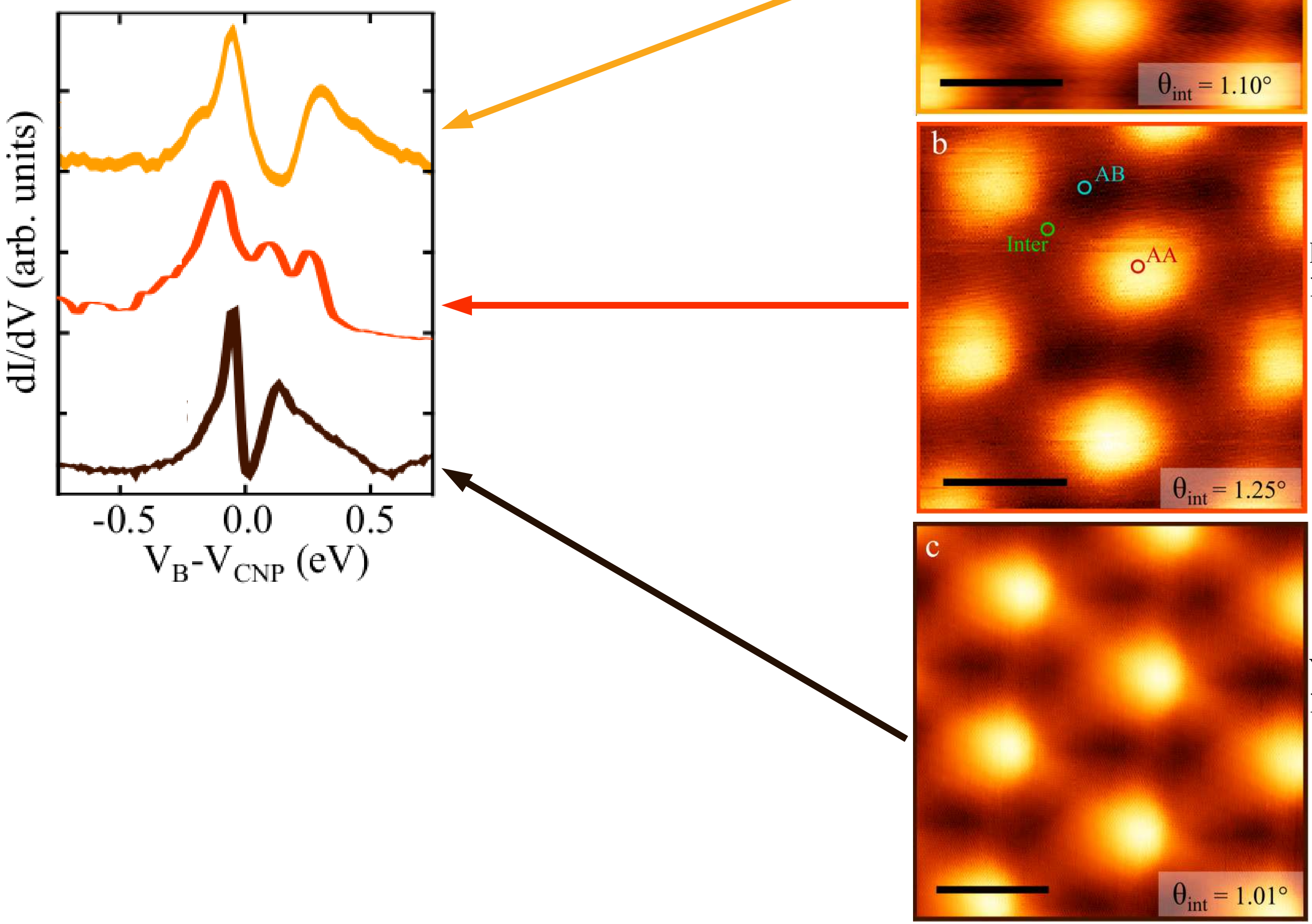
$$\begin{pmatrix} \boldsymbol{k_{b_1}} \\ \boldsymbol{k_{b_2}} \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} \boldsymbol{k_{t_1}} \\ \boldsymbol{k_{t_2}} \end{pmatrix}$$

$$\begin{pmatrix} \boldsymbol{a_{t_1}} \\ \boldsymbol{a_{t_2}} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \boldsymbol{a_{b_1}} \\ \boldsymbol{a_{b_2}} \end{pmatrix}$$

$$\begin{pmatrix} \boldsymbol{a_{t_1}} \\ \boldsymbol{a_{t_2}} \end{pmatrix} = \begin{pmatrix} cos\theta_2 & -sin\theta_2 \\ sin\theta_2 & cos\theta_2 \end{pmatrix} \begin{pmatrix} (\varepsilon_{uni}+1) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} cos\theta_1 & -sin\theta_1 \\ sin\theta_1 & cos\theta_1 \end{pmatrix} \begin{pmatrix} (\varepsilon_{bi}+1) & 0 \\ 0 & (\varepsilon_{bi}+1) \end{pmatrix} \begin{pmatrix} \boldsymbol{a_{b_1}} \\ \boldsymbol{a_{b_2}} \end{pmatrix}$$

$\longrightarrow$ $(\theta, \varepsilon_{uni}, \theta_s, \varepsilon_{bi})$

Heterostrain in experiments



A. Kerelsky et al. Nature 572, 95-100 (2019)

$\varepsilon_{bi} = 0.13\%$

$\varepsilon_{uni} = -0.55\%$

$\theta_s = 34°$

L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)

$\varepsilon_{bi} = -0.06\%$

$\varepsilon_{uni} = 0.35\%$

$\theta_s = 10.6°$

Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

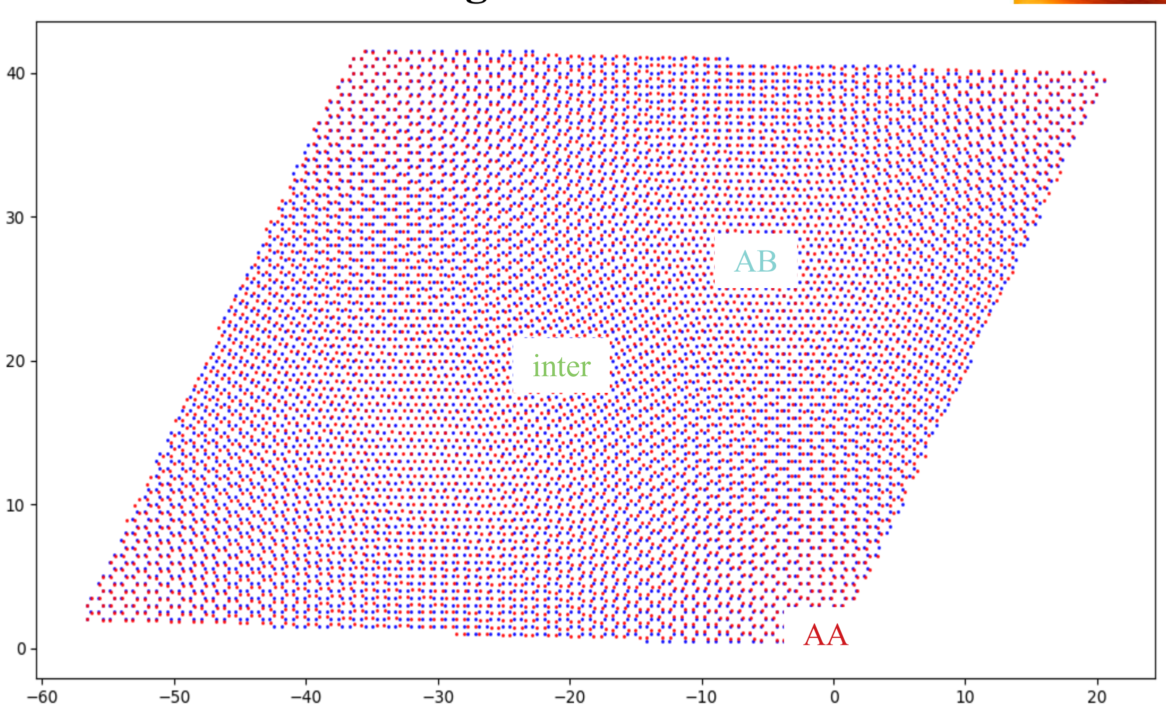
$\varepsilon_{bi} = -0.0\%$

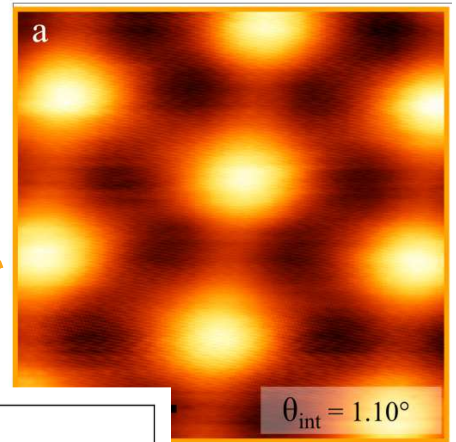
$\varepsilon_{uni} = 0.16\%$

$\theta_s = -26°$

Heterostrain in experiments

Periodic cell including heterostrain



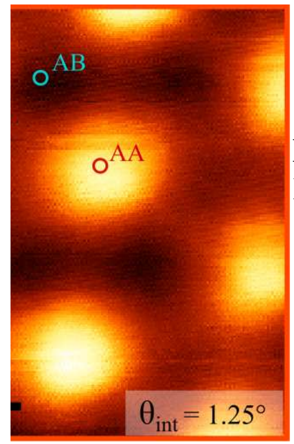


A. Kerelsky et al. Nature 572, 95-100 (2019)

$\varepsilon_{bi} = 0.13\%$

$\varepsilon_{uni} = -0.55\%$

$\theta_s = 34°$

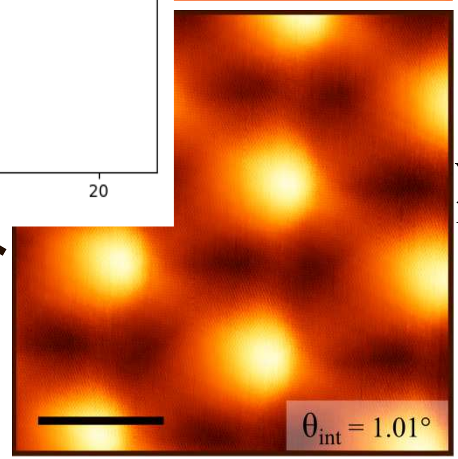


L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)

$\varepsilon_{bi} = -0.06\%$

$\varepsilon_{uni} = 0.35\%$

$\theta_s = 10.6°$



Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

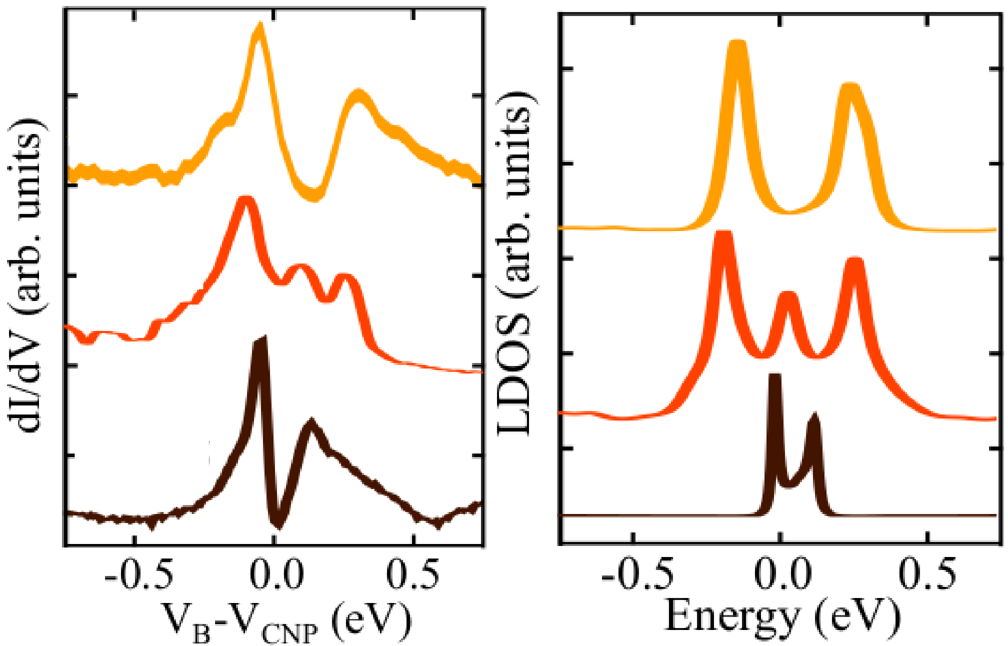
$\varepsilon_{bi} = -0.0\%$

$\varepsilon_{uni} = 0.16\%$

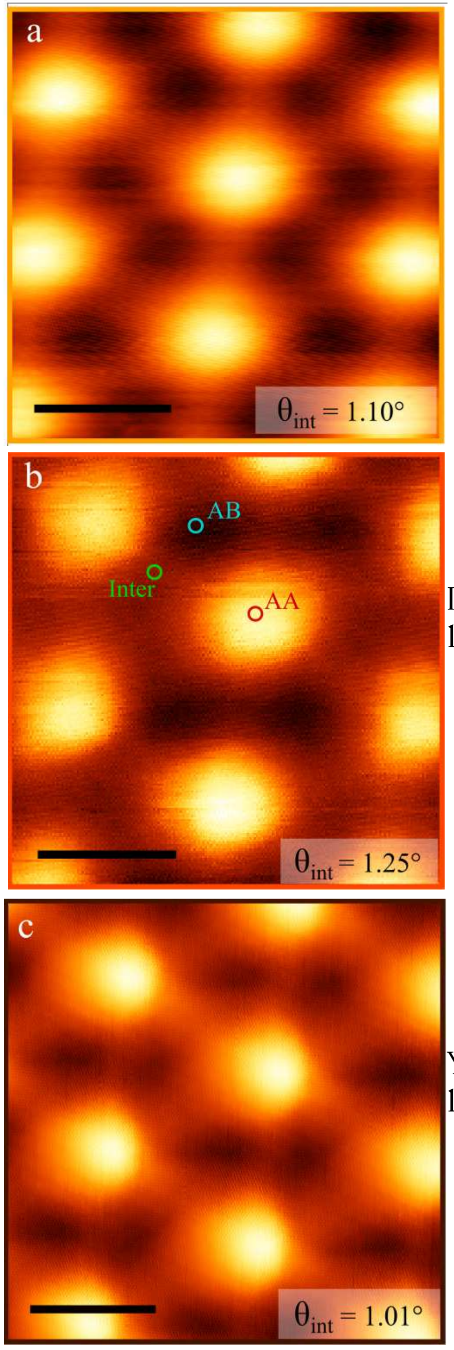
$\theta_s = -26°$

Heterostrain in TB calculations

Tight binding calculations



- By including heterostrain, we describe the physics !



A. Kerelsky et al. Nature 572, 95-100 (2019)

ε_{bi} = 0.13%

ε_{uni} = -0.55%

θ_s = 34°

L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)

ε_{bi} = -0.06%

ε_{uni} = 0.35%

θ_s = 10.6°

Y. Choi et al. Nature Physics 15, 1174-1180 (2019)

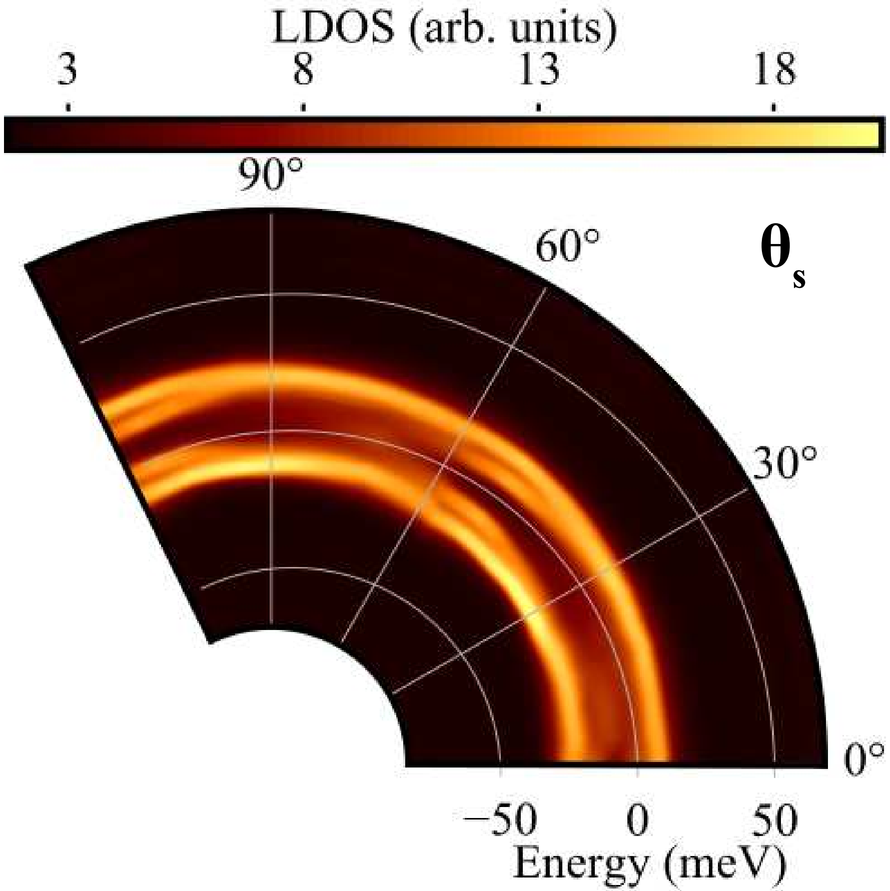
ε_{bi} = -0.0%

ε_{uni} = 0.16%

θ_s = -26°

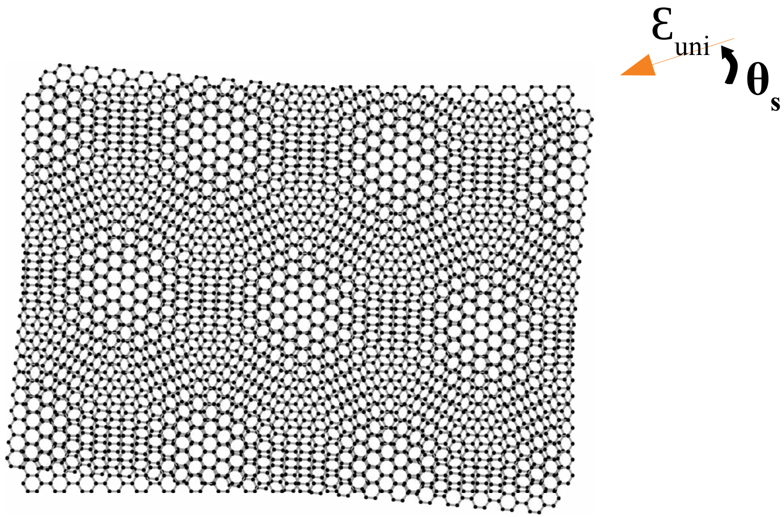
Heterostrain in TB calculations

$\theta = 1.1°$
$\varepsilon_{uni} = 0.4\ \%$



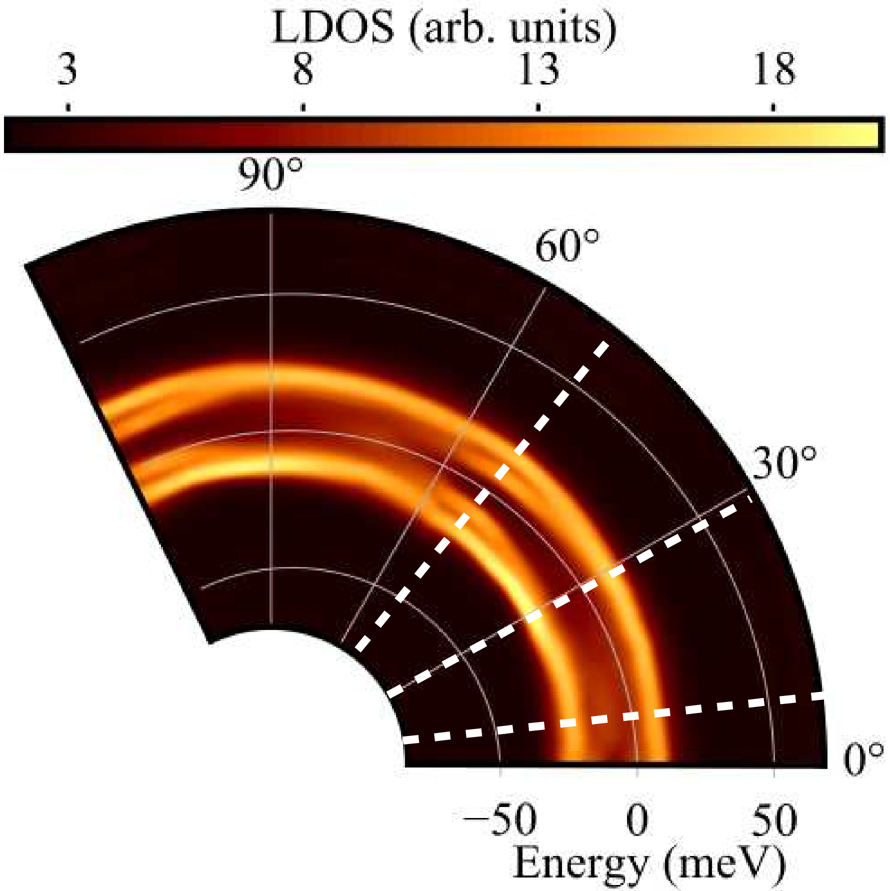
Tight binding calculations
Ahmed Missaoui
Guy Trambly de Laissardière
LPTM Cergy Pontoise

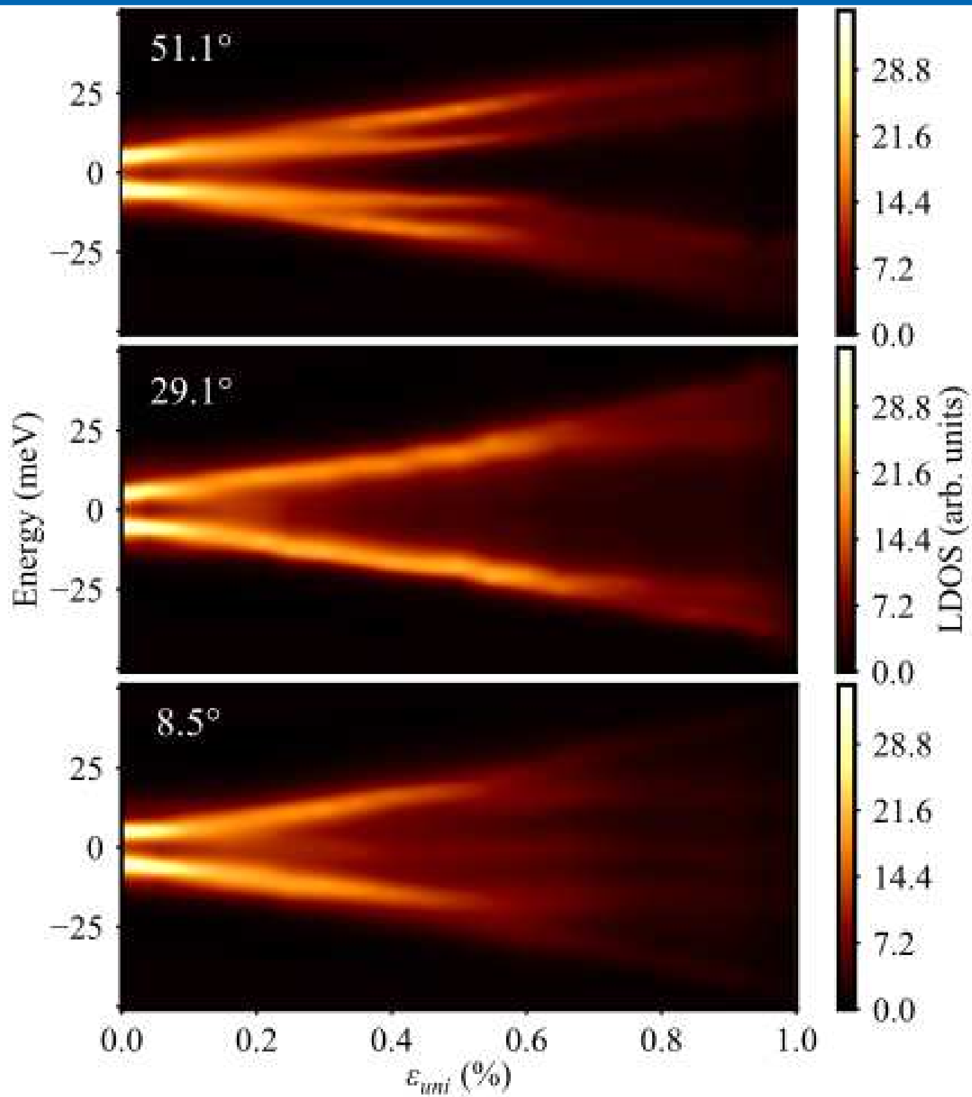
UNIVERSITÉ de Cergy-Pontoise



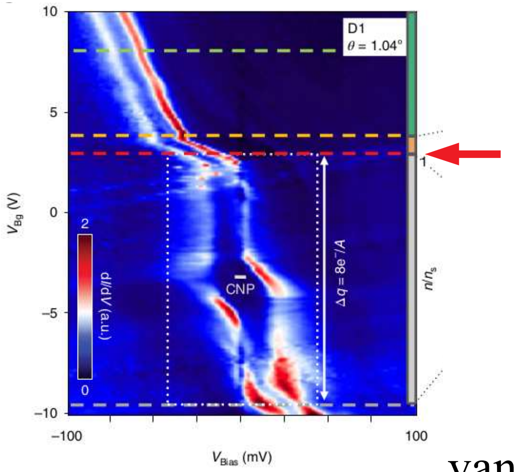
Heterostrain in TB calculations

θ = 1.1°
ε_{uni} = 0.4 %



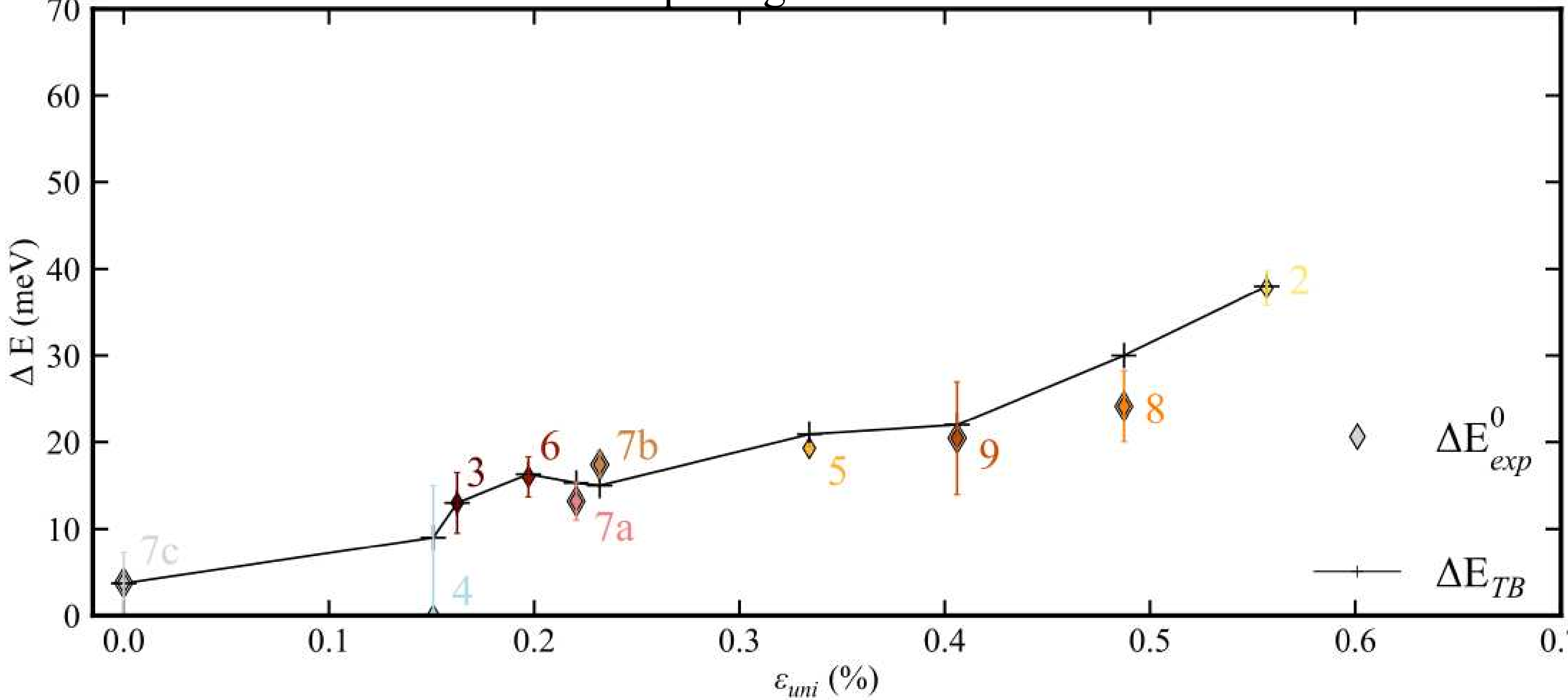


Meta-analysis

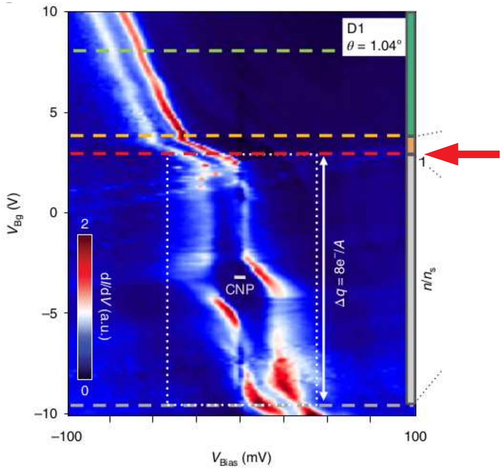


1. L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)
2. A. Kerelsky et al. Nature 572, 95-100 (2019)
3. Y. Choi et al. Nature Physics 15, 1174-1180 (2019)
4. Y. Jiang et al. Nature 573, 91-95 (2019)
5. Y. Xie et al. Nature 572, 101-105 (2019)
6. Z. Zhang et al. Phys. Rev. Research 2, 033181 (2020)
7. D. Wong et al. Nature 582(7811), 198-202 (2020)
8. Y. Choi et al. arXiv 2008.11746 (2020)
9. K. P. Nuckolls et al. arXiv 2007.03810 (2020)

van Hove spacing as a function of strain



Meta-analysis



1. L. Huder et al. Phys. Rev. Lett. 120, 156405 (2018)
2. A. Kerelsky et al. Nature 572, 95-100 (2019)
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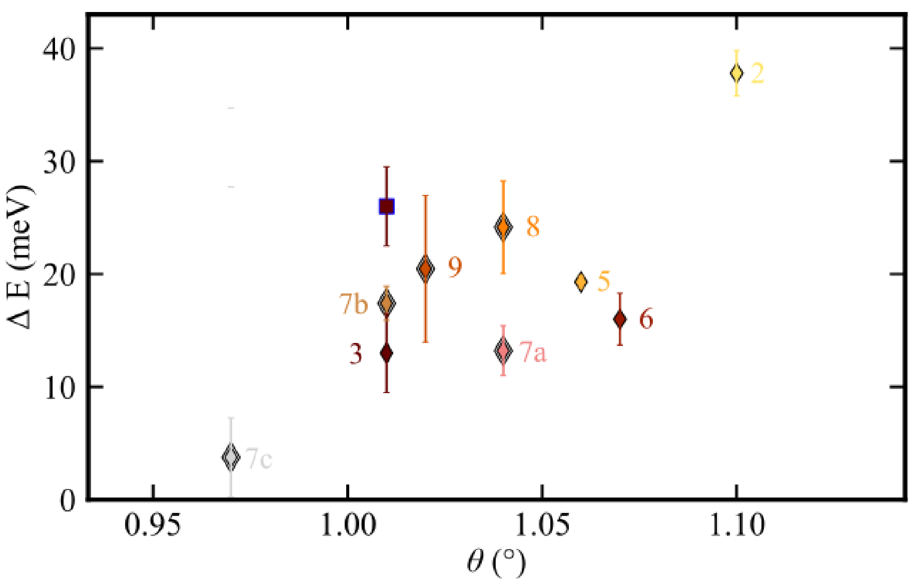
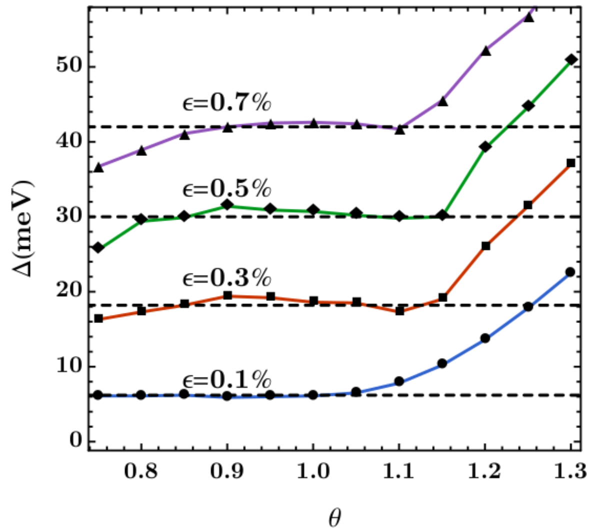
8. Y. Choi et al. arXiv 2008.11746 (2020)
9. K. P. Nuckolls et al. arXiv 2007.03810 (2020)

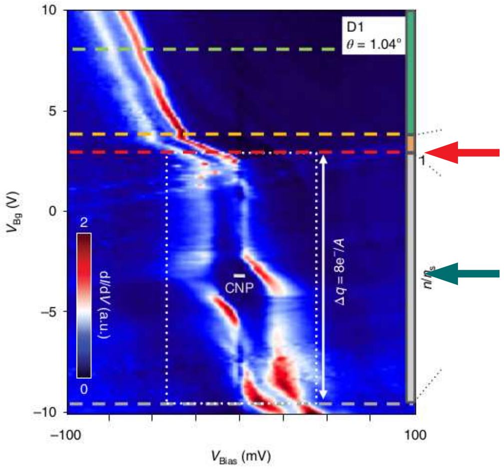
van Hove spacing as a function of twist angle





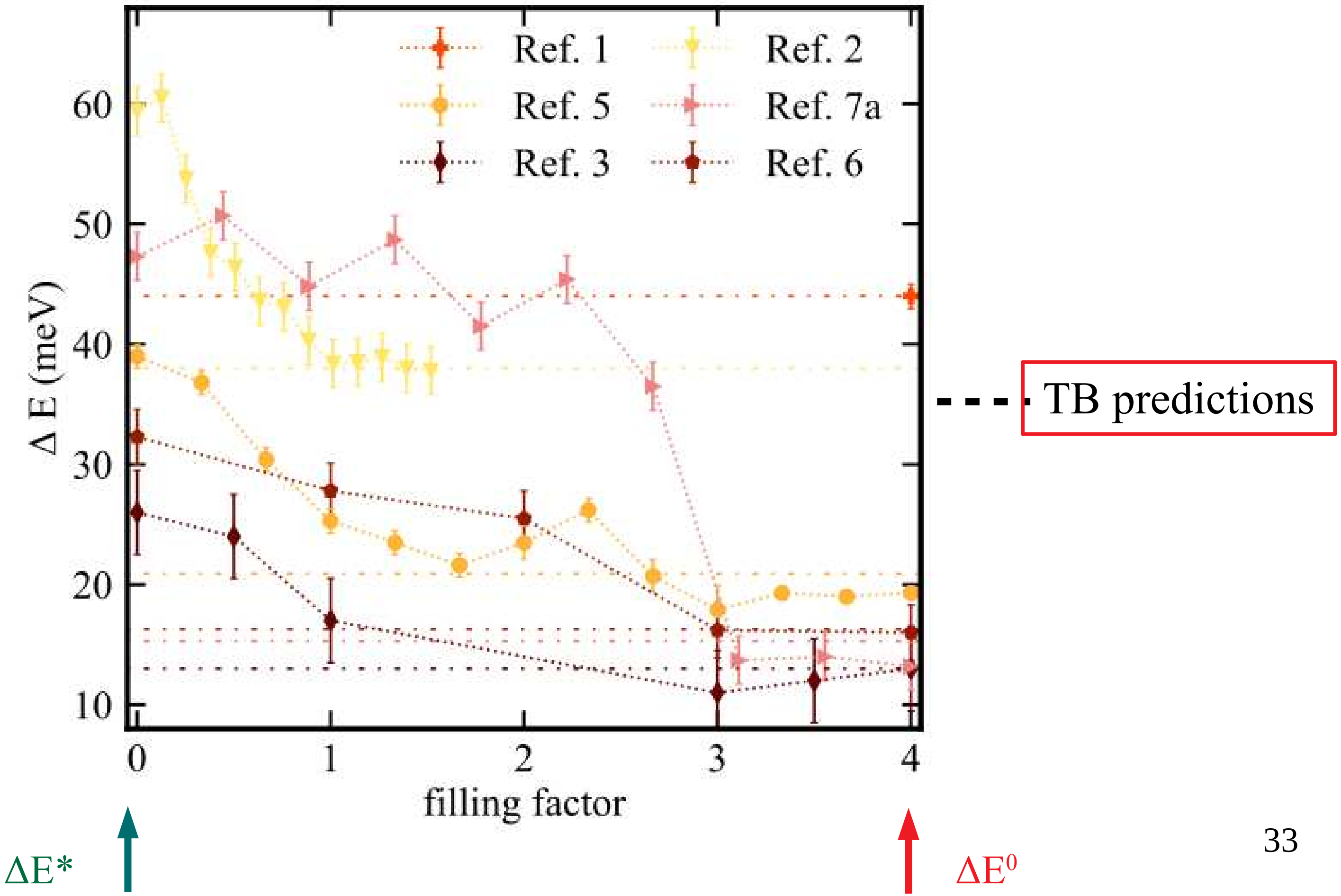
Z. Bi, N. F. Q. Yuan, and L. Fu. Phys. Rev. B 100, 035448 (2019)

Meta-analysis

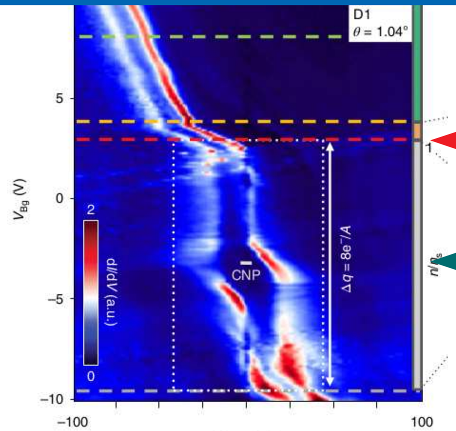


$$\frac{E_C}{E_k} \to \infty$$

van Hove spacing as a function of doping

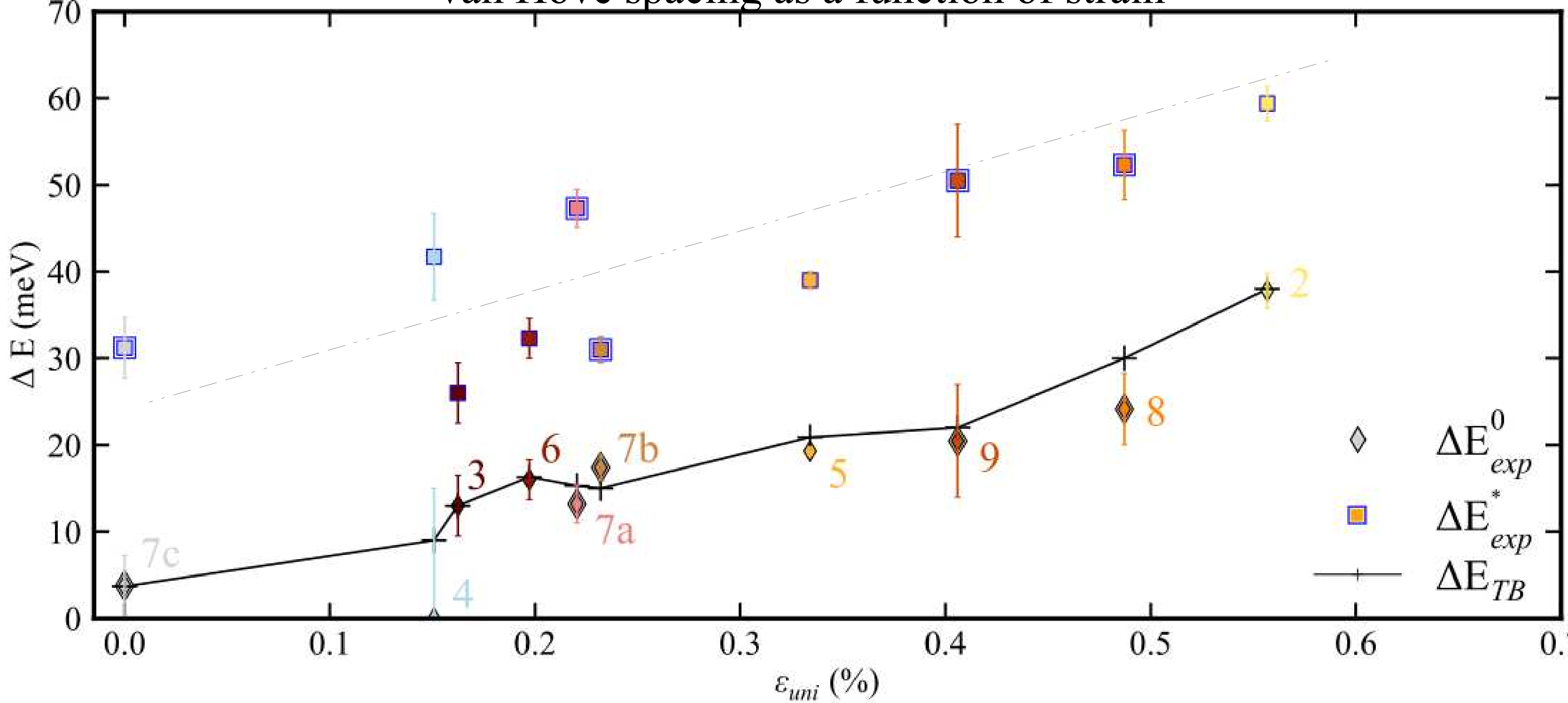


Meta-analysis



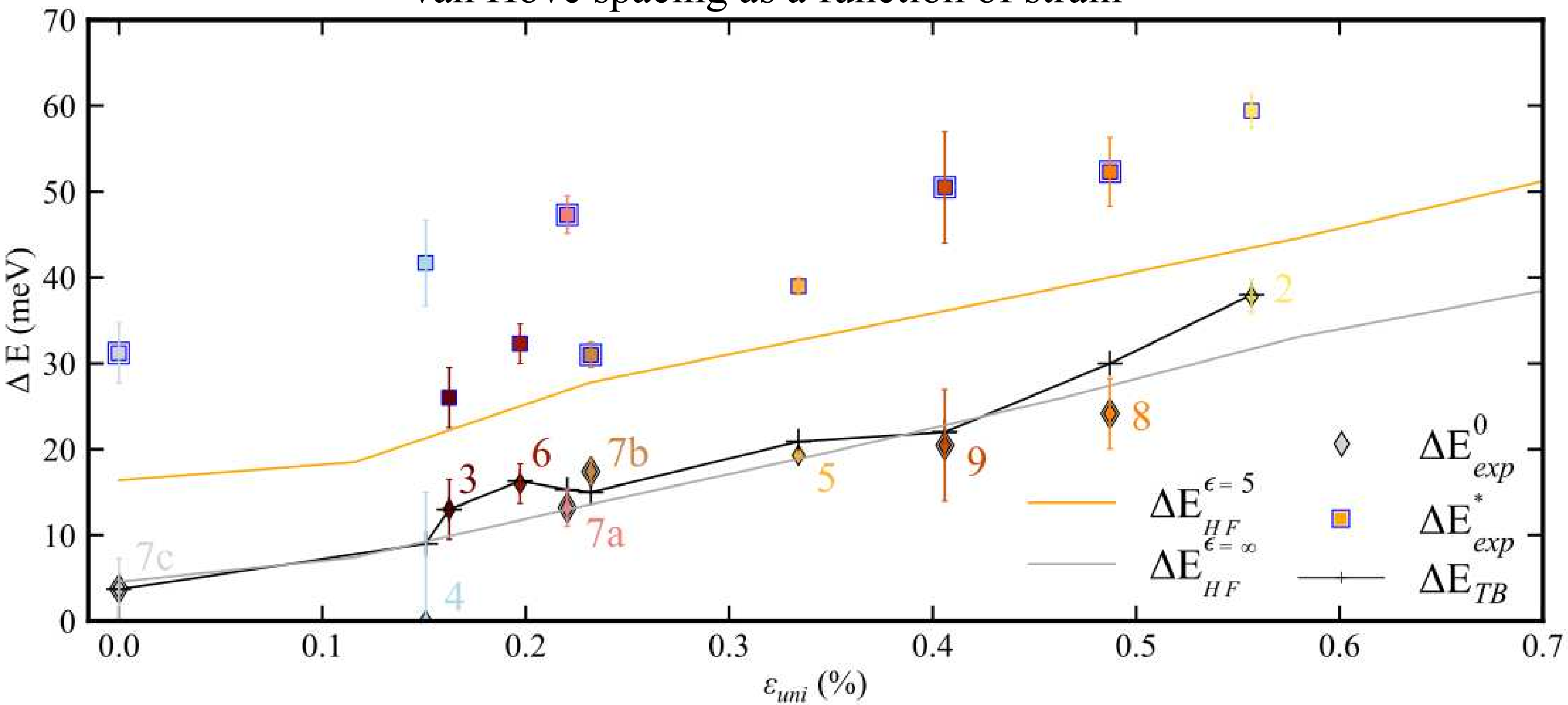
→ Need to include interactions

van Hove spacing as a function of strain

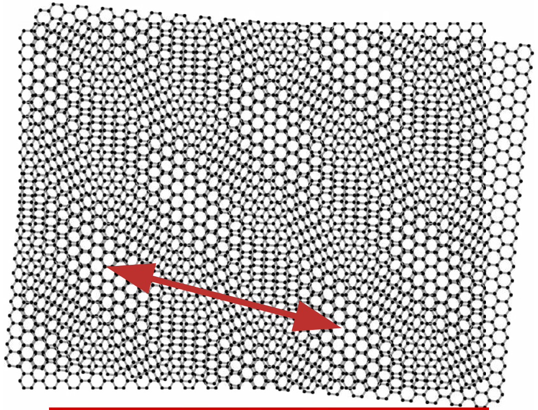


Hartree-Fock
Continuum calculations
Tommaso Cea
Paco Guinea
IMDEA Nanosciencia

van Hove spacing as a function of strain

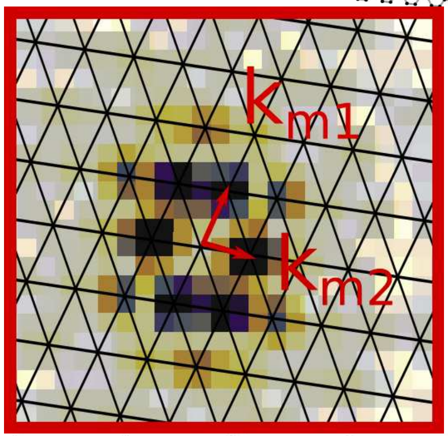


Take home message

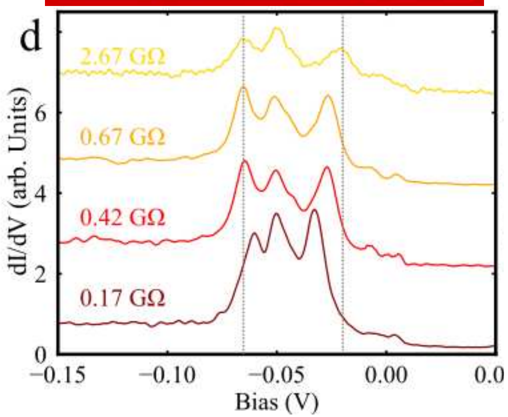


→ The physics of TBLG near magic angle are controlled by strain, not by interlayer angle.

N. Nakatsuji, M. Koshino, arXiV (2022)



→ Efficient method to extract « average » strain from STM images



→ Motivation to further investigate the complex parameter space that controls the physics at play *(tip induced strain, inhomogeneous strain, electrostatic environement, local tip doping, ...)*