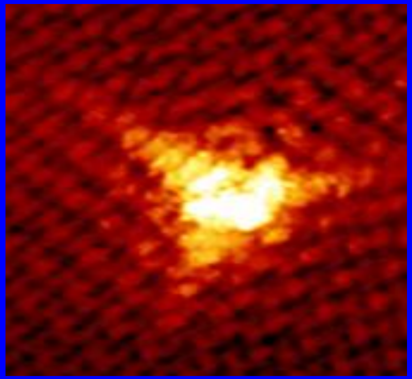
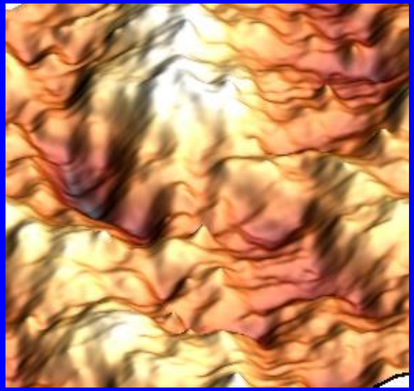
Interaction of Dirac electrons with spins and point charges

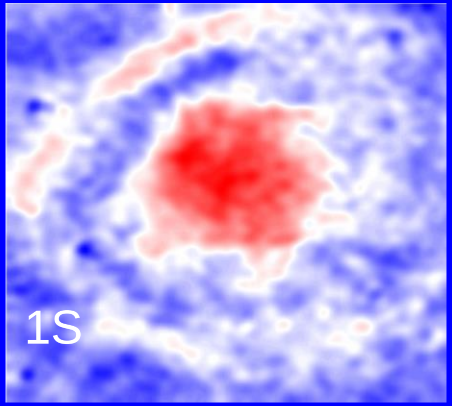
Vacancies in graphene



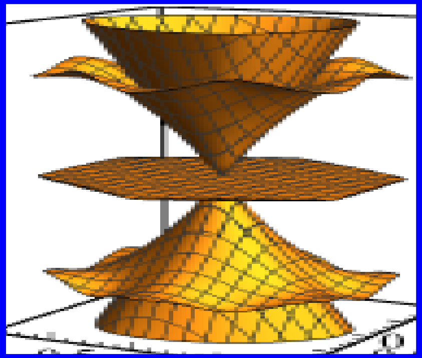
Vacancy Magnetic moment and Kondo screening



Vacancy Charge and Tunable artificial atom



Twisted bilayer graphene



Eva Y. Andrei

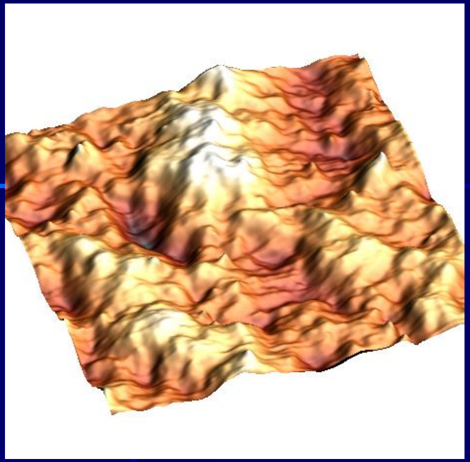
LECTURE NOTES POSTED AT:

http://www.physics.rutgers.edu/~eandrei/links.html#trieste18

Summer School on Collective Behaviour in Quantum Matter

ICTP

Scanning tunneling microscopy and spectroscopy

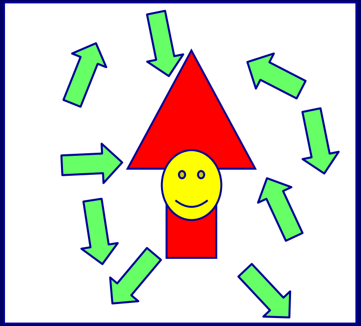


- Engineering electronic properties
  - Density of states and Landau levels in graphene
  - Scanning tunneling microscopy (STM) and spectroscopy (STS)
  - Defects:
    Atomic collapse and artificial atom
    Kondo effect
  - Substrate:
    Twisted graphene

Kondo Screening of Impurity Moments in Metals

$T>T_K$

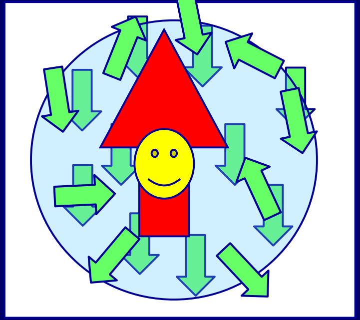
Unscreened



J antiferromagnetic coupling to electron bath

$T<T_K$

Screened



Kondo cloud

$$T_K \propto \exp(-1/\rho J)$$

ρ ***density of states at*** $\boldsymbol{E_F}$

$\rho(E_F) > 0$, $J>0 \mapsto T_K > 0$

- Normal metals $\rho(E_F) \sim finite; J \neq 0$ $\mapsto T_K > 0$
- Insulators $\rho(E_F) = 0$ No Kondo screening

What happens in a pseudogap system?

Kondo Screening in pseudo-gap systems

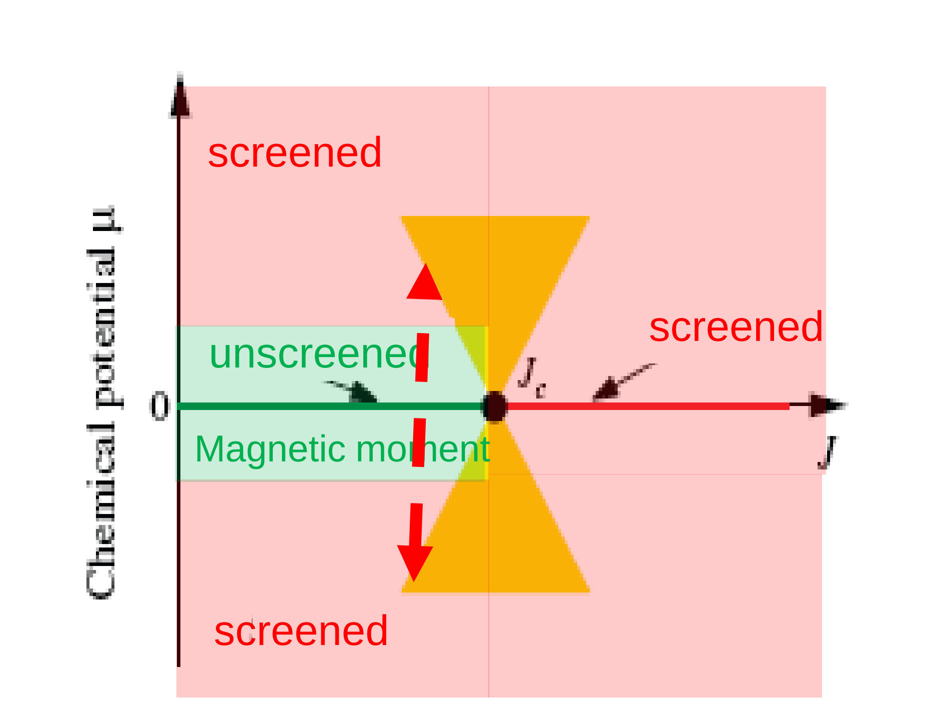
- Pseudo- gap systems $\rho(E) \propto E^r$ screening suppressed.
  - r = 1 (graphene, high T_c superconductors)

μ~0 (undoped)

- Kondo screening only for J>Jc
- J_c finite only for asymmetric DOS

|μ|>>0 doped

- Normal Kondo screening

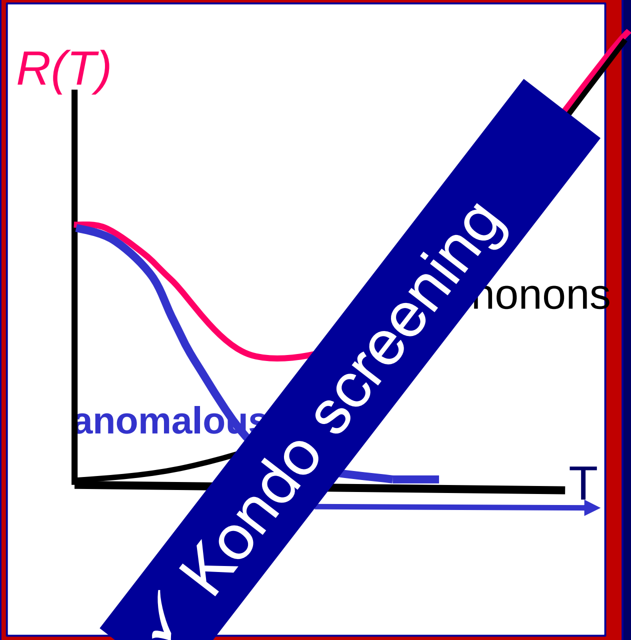


- D. Withoff and E. Fradkin, Phys. Rev. Lett. 64, 1835(1990)
- K. Chen and C. Jayaprakash, J. Phys L491 (1995)
- K. Ingersent, Phys. Rev. B54, 11936 (1996)
- C. Cassanello and E. Fradkin , (1996)
- R. Bulla, T. Pruschke, and A. C. Hewson, (1998)
- Polkovnikov A., Phys. Rev. B, 65 (2002) 064503
- Vojta M. and Fritz L., Phys. Rev. B, 70 (2004) 094502.
- Vojta, Fritz, Bulla EPL (2010)
- PW Lo, GY Guo, F. Anders, arXiv:1402.0040

Electrical tuning of magnetic moment

Kondo Screening Experimental Signatures

Resistance minimum



✓ Kondo screening

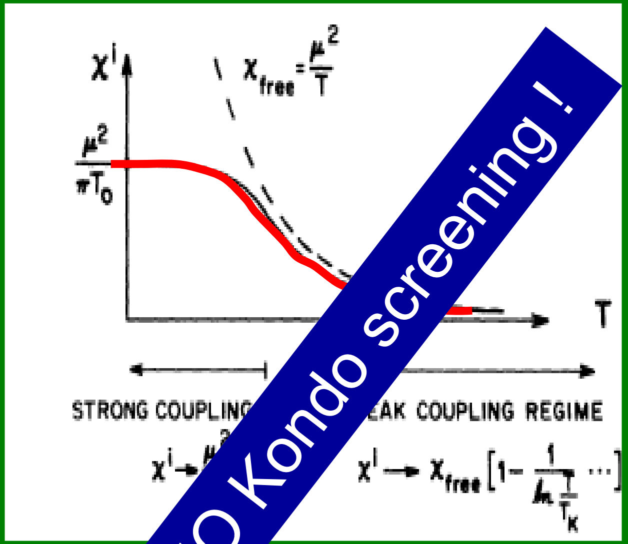
nature physics | LETTER
PUBLISHED ONLINE: 3 APRIL 2011 | DOI:10.1038/NPHYS1

Tunable Kondo effect in graphene with defects

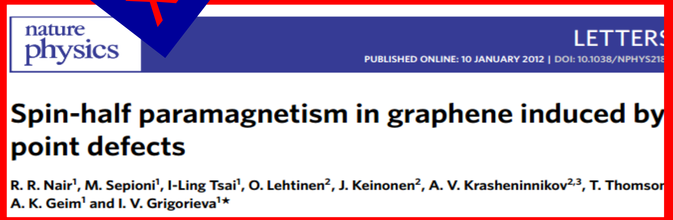
Jian-Hao Chen[1,2†], Liang Li[2], William G. Cullen[1,2], Ellen D. Williams[1,2] and Michael S. Fuhrer[1,2★]

Measures:
scattering off Kondo cloud

Magnetization saturation



✗ NO Kondo screening !



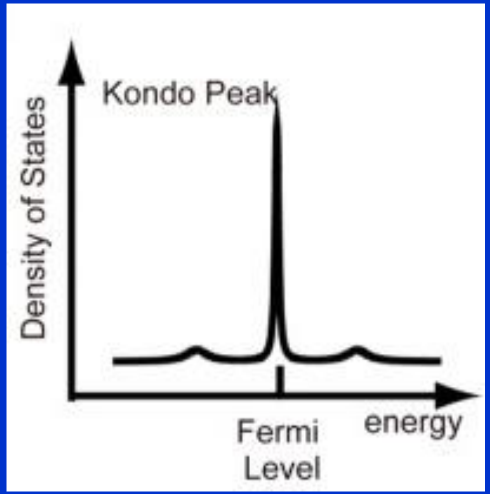
nature physics | LETTERS
PUBLISHED ONLINE: 10 JANUARY 2012 | DOI: 10.1038/NPHYS218

Spin-half paramagnetism in graphene induced by point defects

R. R. Nair[1], M. Sepioni[1], I-Ling Tsai[1], O. Lehtinen[2], J. Keinonen[2], A. V. Krasheninnikov[2,3], T. Thomson A. K. Geim[1] and I. V. Grigorieva[1★]

Measures:
Unscreened moment

DOS – Kondo Peak



- Kondo Peak at E_F
- Low T linewidth Γ

$$k_B T_K \sim \Gamma/2$$

DOS enhancement at E_F

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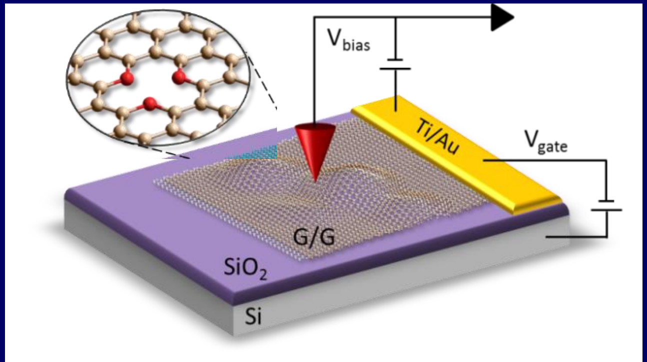
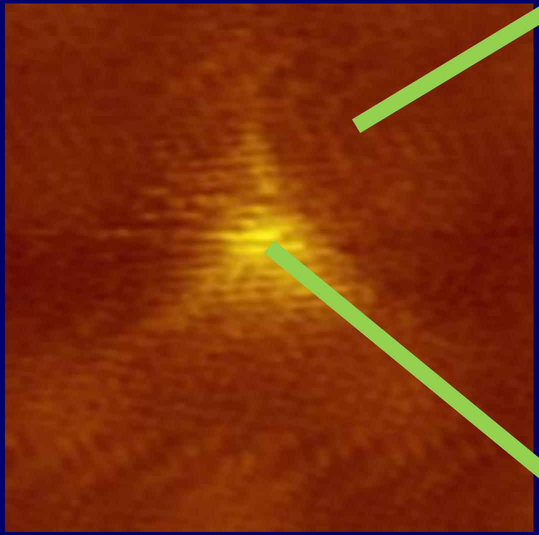
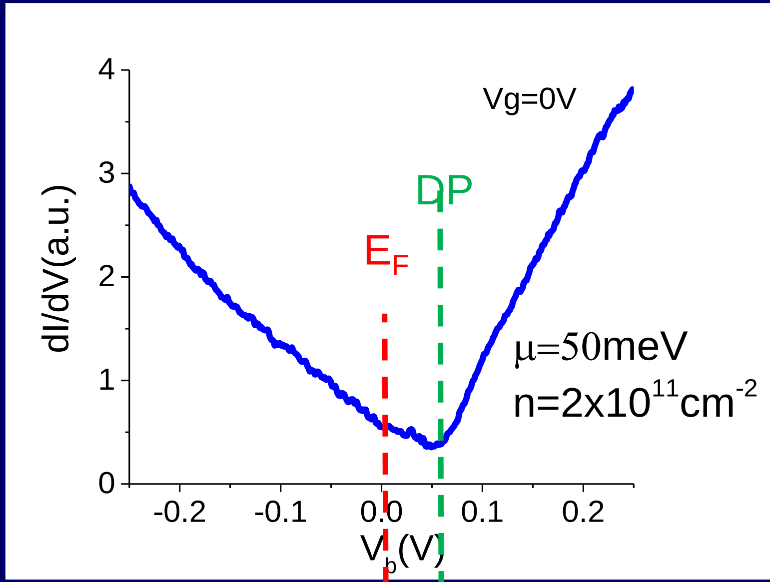
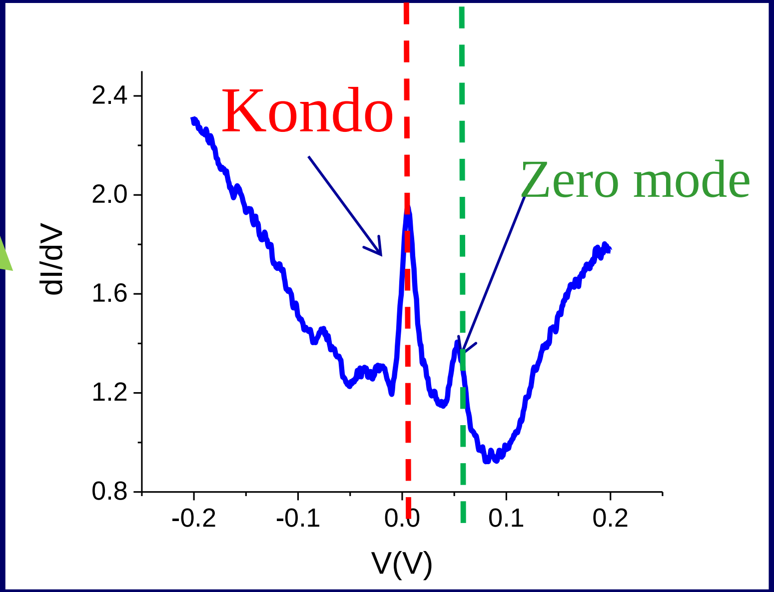
Vacancy in graphene









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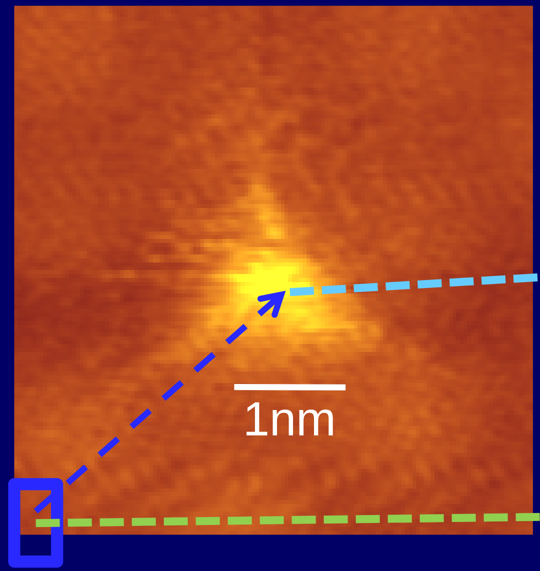
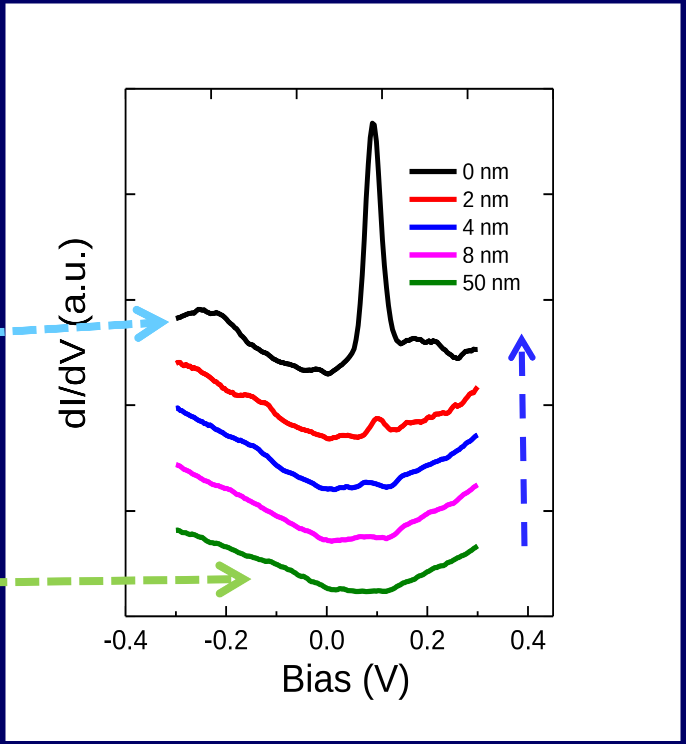
Vacancy Peak

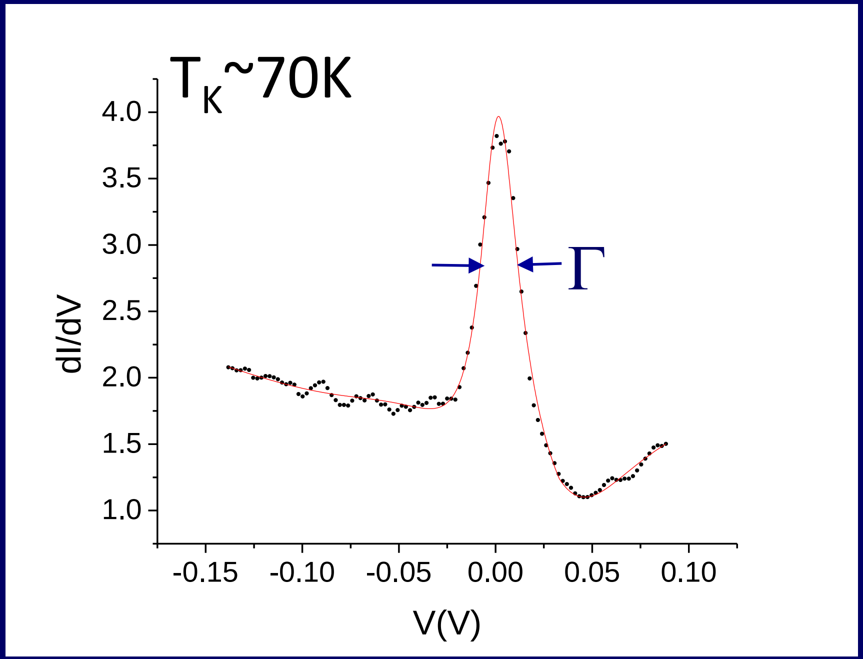


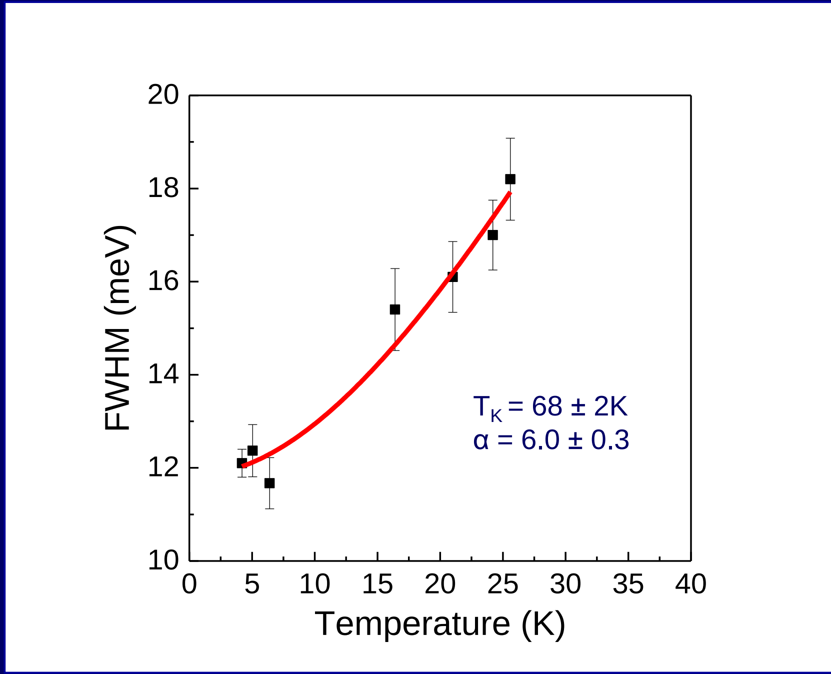


Vacancy Peak

- localized on vacancy site <2nm.
- pinned to the Dirac point

Kondo Temperature





Fit to Fano lineshape

$$\frac{dI(V)}{dV} = A\frac{(\varepsilon + q)^2}{1 + \varepsilon^2} + B$$

Fit to T dependence

$$\Gamma = \sqrt{(\alpha k_B T)^2 + (2k_B T_K)^2}$$

$$\varepsilon = \frac{E - \varepsilon_0}{\Gamma/2}$$

$$k_B T_K \sim \Gamma/2$$

O. Újsághy, et al. Solid State Commun. **117**, 167(2001)
A.S. Zyazin, et al. Synthetic Metals **161**, 591 (2010)
M. Ternes, *et.al.* J. Phys.: Condens. Matter 21, 053001, (2009)

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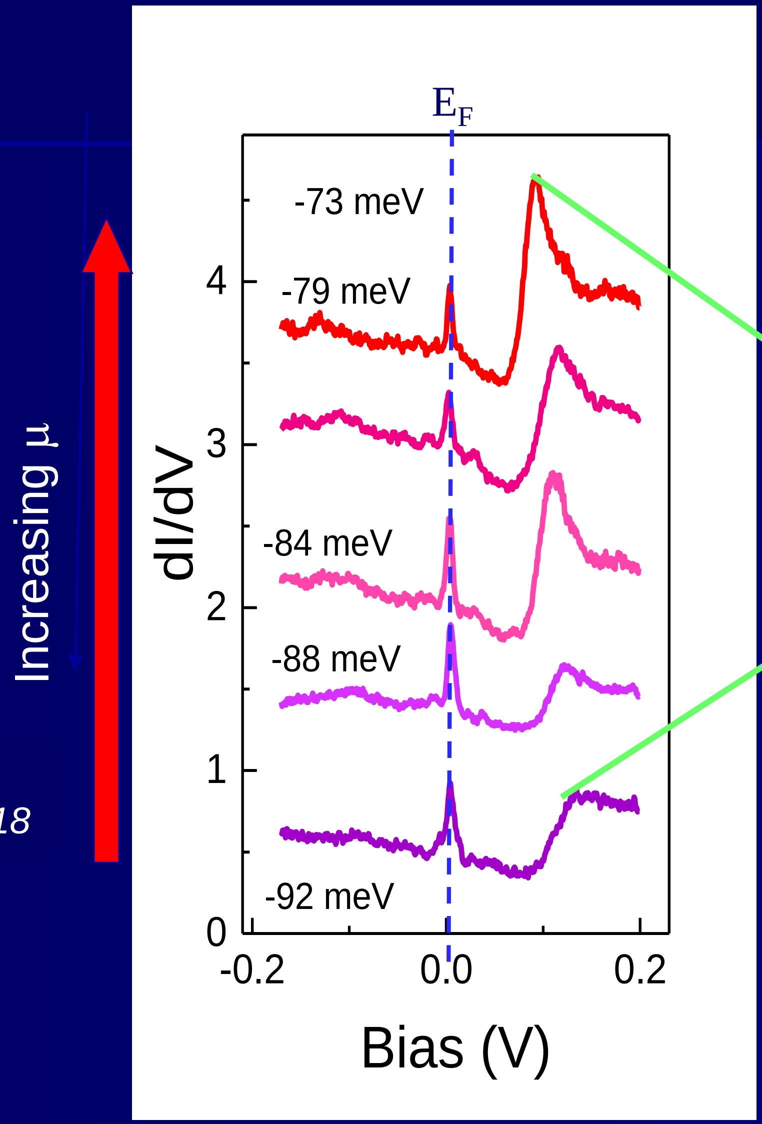
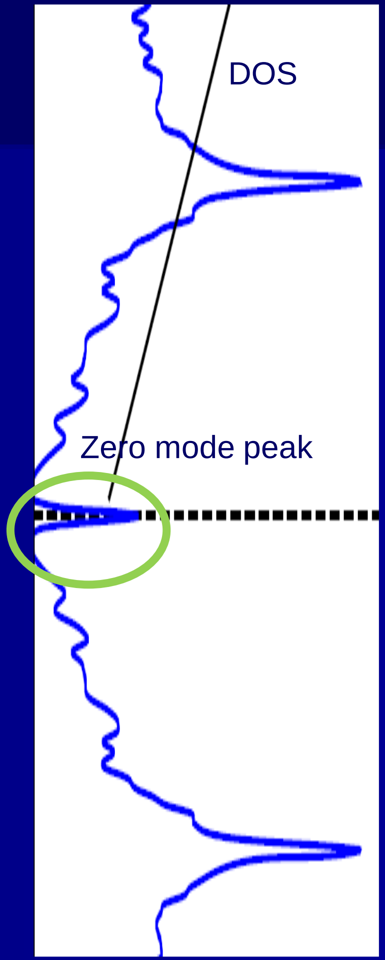
Gate Dependence

Kondo Peak



Pinned to E_F

Zero mode



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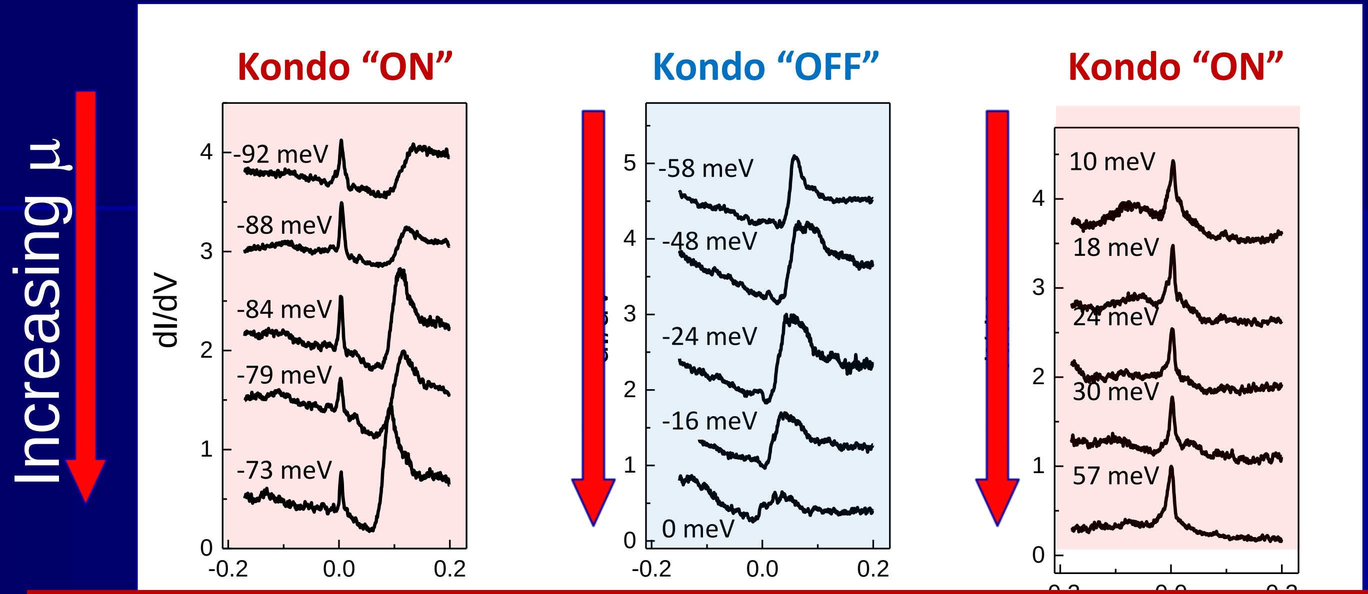
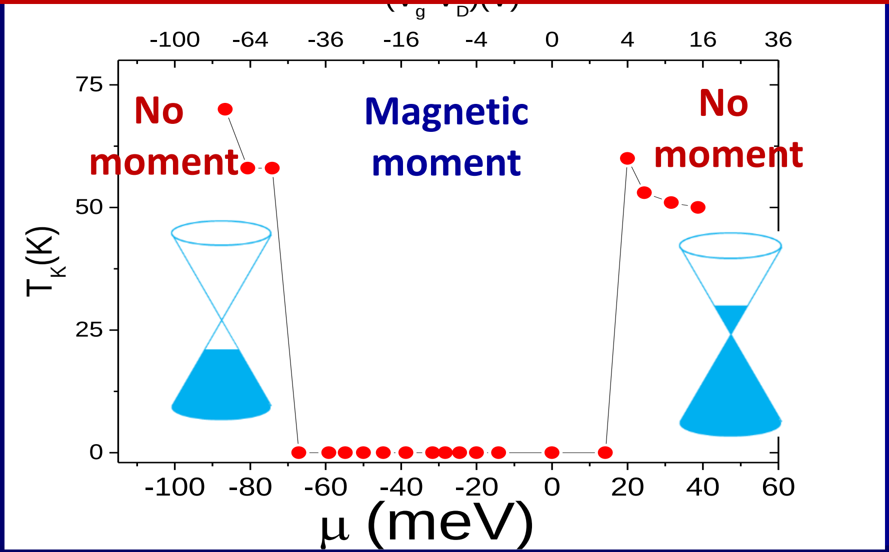
Reentrant Kondo Screening



Electrically tuned magnetic moment



$J<J_c$

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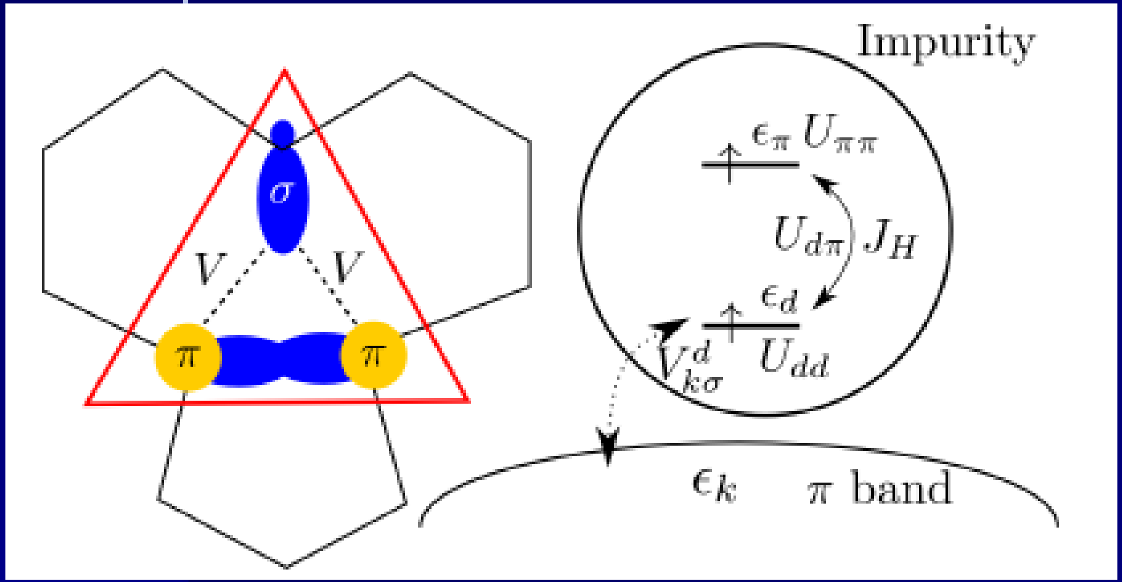
Model for Kondo screening of vacancy moment

- Anderson impurity model
- Numerical renormalization group calculations



• bare σ-orbital energy	$\varepsilon_d = -1.6eV$
• On site Coulomb	$U_{dd} = 2eV$
• Exchange coupling	$U_{d\pi} = 0.1eV$
• Hund coupling	$J_H \sim -0.35eV$
• Critical coupling	$\Gamma_c = 1.15eV$

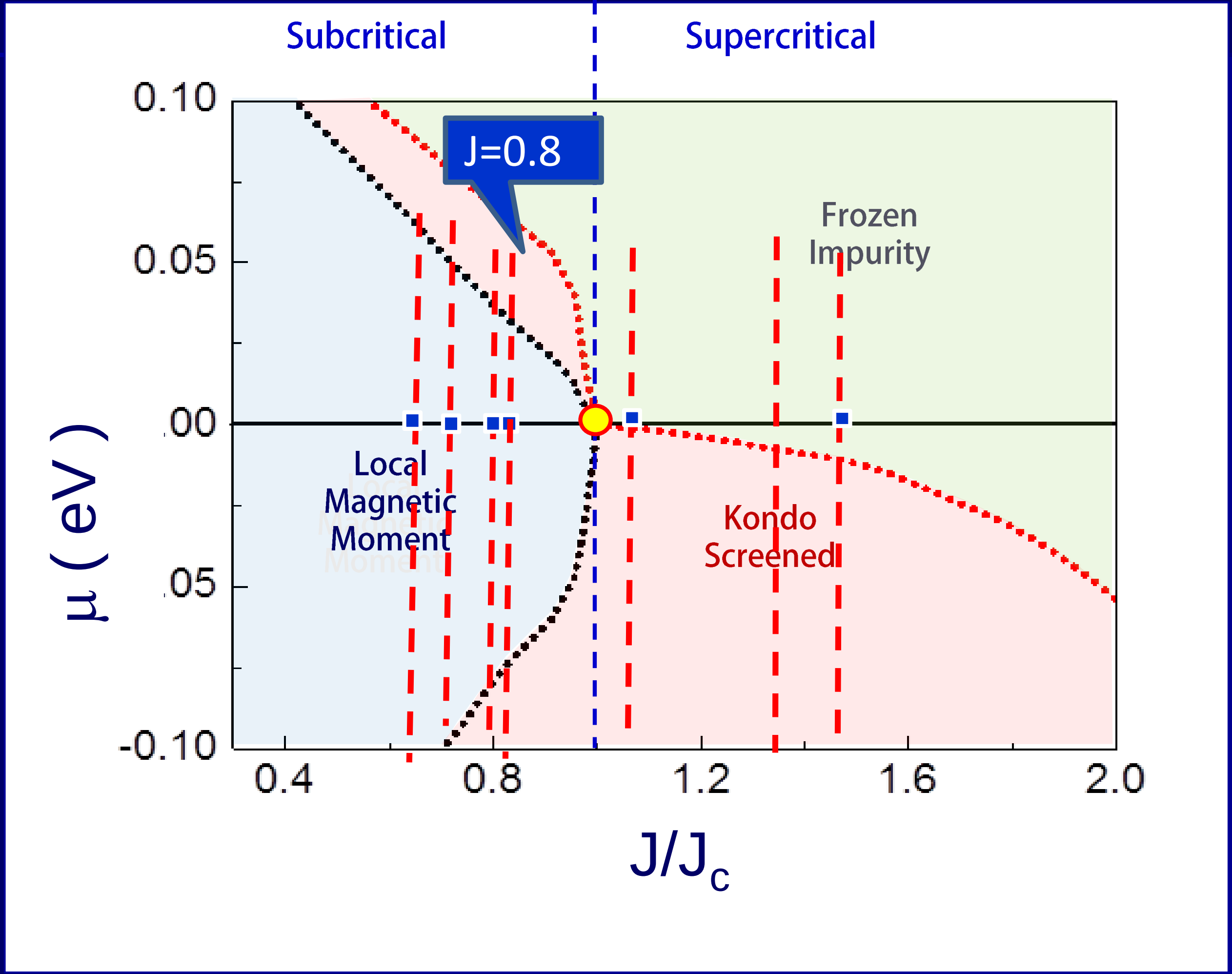
Single orbital approximation:
$$U_{eff}(\mu) = \begin{cases} U_{dd} & \mu \le 0 \\ U_{dd} + \min(U_{d\pi}, \alpha\mu) & \mu > 0 \end{cases}$$

D. May et al Phys. Rev. B 97, 155419 (2018)

Y Jiang et al Nature Communications 2018
J. Mao et al arXiv:1711.06942 (2017)

Kondo Screening Phase Diagram

Numerical Renormalization Group

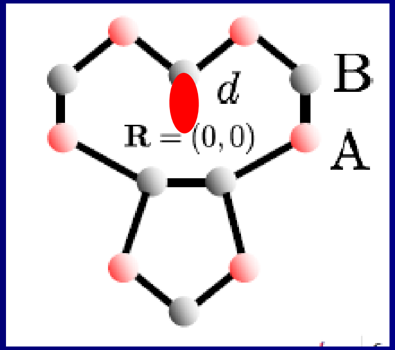


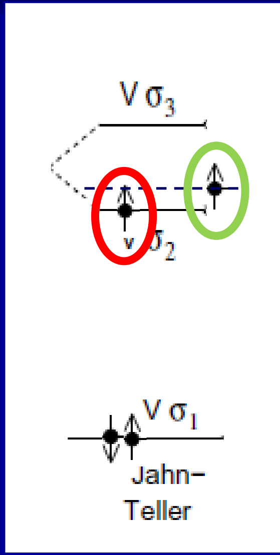
D. May et al Phys. Rev. B 97, 155419 (2018)

Y Jiang et al Nature Communications 2018
J. Mao et al arXiv:1711.06942 (2017)

What determines J?

- σ Dangling bond ↦ localized state ↦ $1\mu_B$





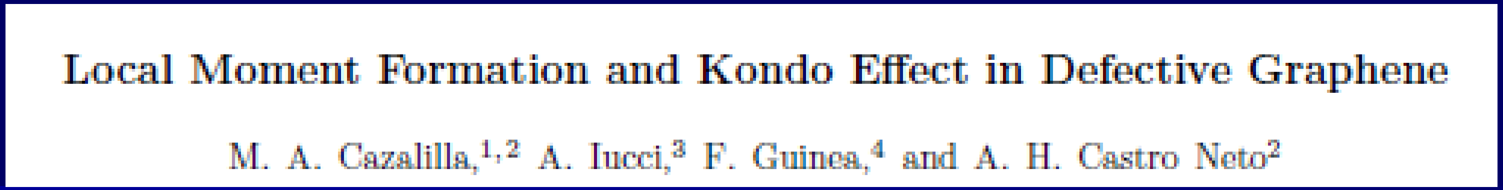
➢ σ state (in plane) – orthogonal to π conduction electrons ↦J=0

➢ p_z state – Ferromagnetic coupling ↦ J=0

J=0 ↦ NO KONDO SCREENING !!

Hentschel, M. & Guinea, F*Phys Rev B* **76**, 115407 (200)7
Haase, P., Fuchs, S., Pruschke, T., Ochoa, H. & Guinea, F (2011)
Cazalilla, M. A. I., A.; Guinea, F.; Castro Neto, A. H (2012)

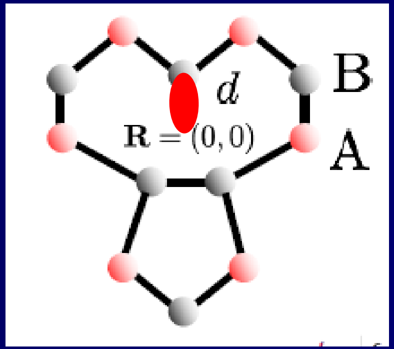
Can J be Finite in Graphene?

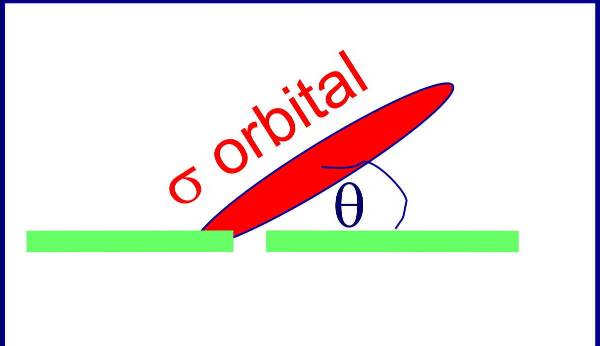

Local Moment Formation and Kondo Effect in Defective Graphene

M. A. Cazalilla,[1,2] A. Iucci,[3] F. Guinea,[4] and A. H. Castro Neto[2]

- Out of plane distortion of dangling bond

$\mapsto$ Finite AF coupling with conduction electrons $\mapsto$ Kondo screening





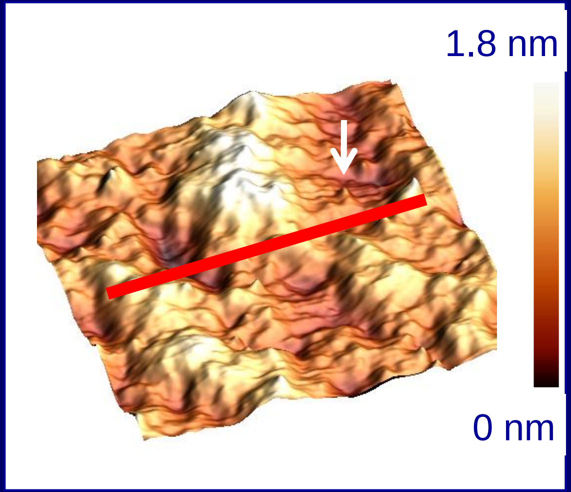
$J \sim \sin\theta$

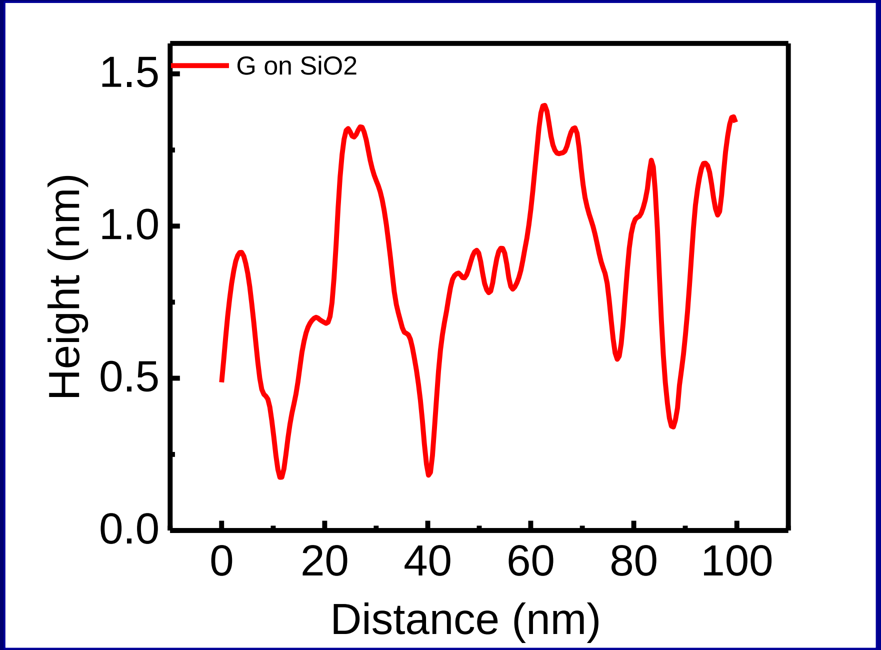
Finite Kondo coupling

Corrugated Substrate ??

Substrate corrugation and Kondo screening

Substrate Corrugation	G/SiO_2 2nm
Maximum T_K	T_K~180K
% of screened vacancies	Most





J. Mao et al
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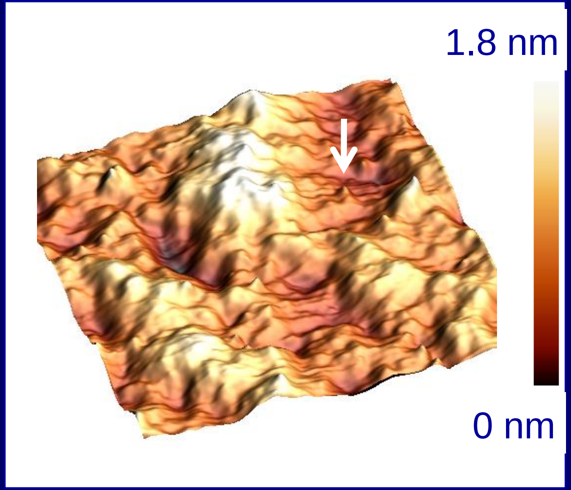
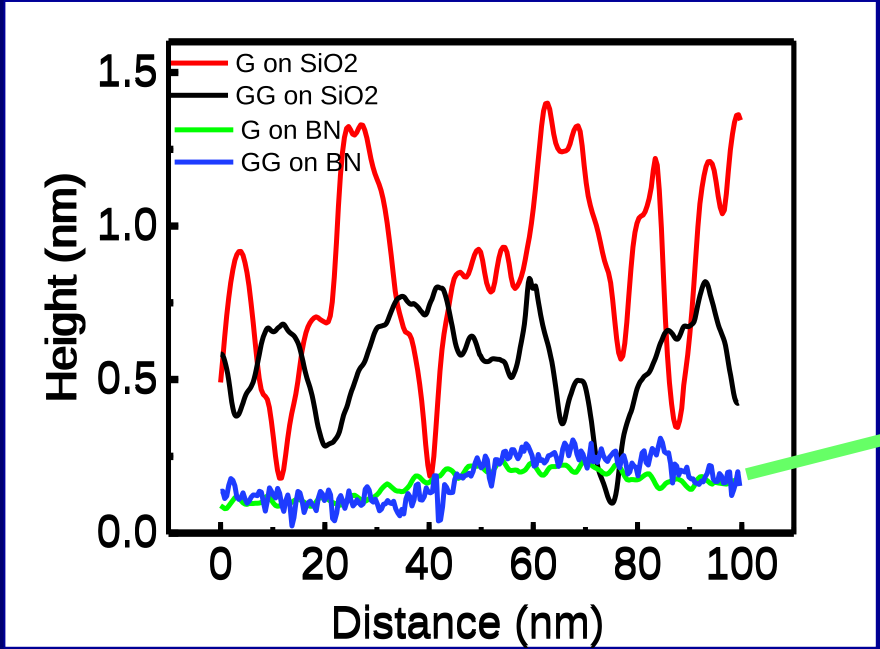
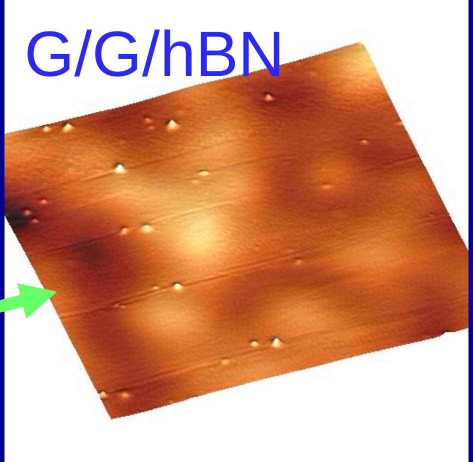
Substrate corrugation and Kondo screening

Substrate Corrugation	G/SiO_2 2nm	$G/G/SiO_2$ 1nm	G/hBN 0.2nm	G/G/hBN 0.2nm
Maximum T_K	T_K~180K	T_K~ 70K	No Kondo	No Kondo
% of screened vacancies	Most	30%	none	none







J depends on Local corrugation

↦ Mechanically controlled magnetism

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Global Measurements and Conflicting results

nature physics — LETTERS

PUBLISHED ONLINE: 3 APRIL 2011 | DOI: 10.1038/NPHYS1962

Tunable Kondo effect in graphene with defects

Jian-Hao Chen[1,2†], Liang Li[2], William G. Cullen[1,2], Ellen D. Williams[1,2] and Michael S. Fuhrer[1,2]*

- R(T) $\mapsto$ Kondo screening
  - ➢ T_K 20-70K

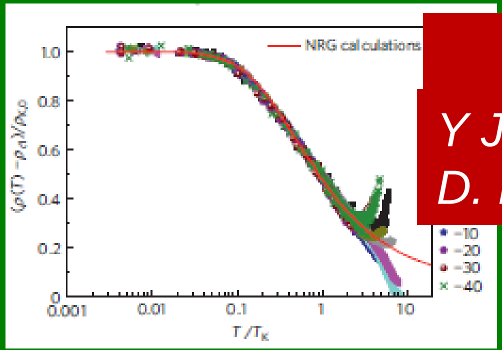
nature physics — LETTERS

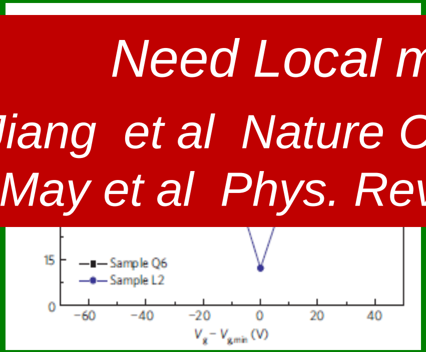
PUBLISHED ONLINE: 10 JANUARY 2012 | DOI: 10.1038/NPHYS2183

Spin-half paramagnetism in graphene induced by point defects

R. R. Nair[1], M. Sepioni[1], I-Ling Tsai[1], O. Lehtinen[2], J. Keinonen[2], A. V. Krasheninnikov[2,3], T. Thomson[1], A. K. Geim[1] and I. V. Grigorieva[1]*

- $\chi(T) \mapsto$ No Kondo screening
- Moments unscreened at low T

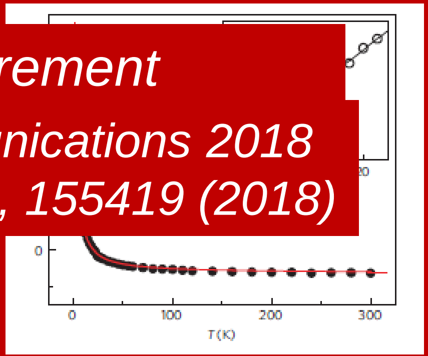


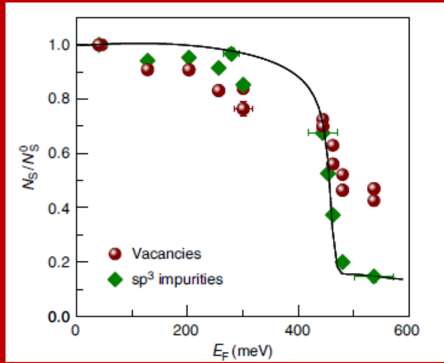


Need Local measurement

Y Jiang et al Nature Communications 2018

D. May et al Phys. Rev. B 97, 155419 (2018)





Measures:

Scattering off Kondo cloud

➢ Sensitive to screened Moments only.

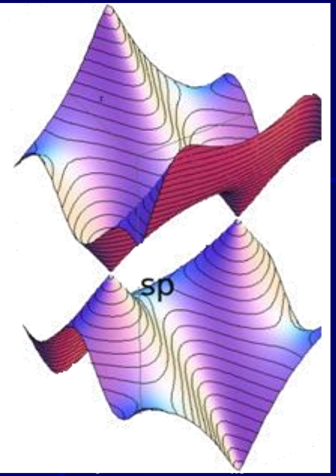
Measures:

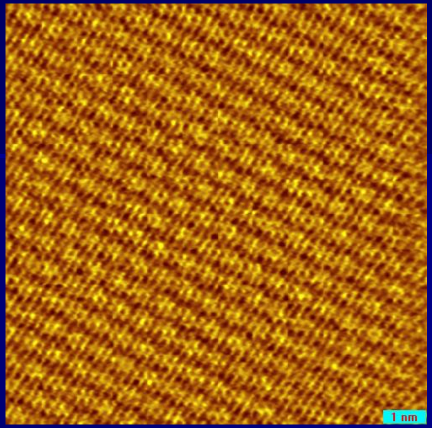
Magnetic moments

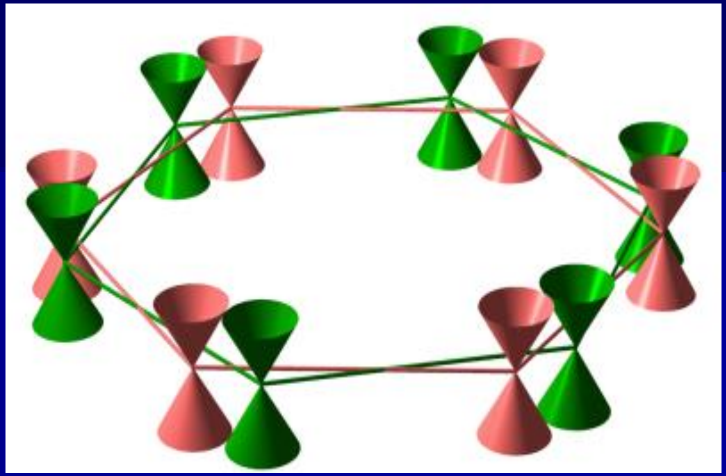
➢ Sensitive to unscreened Moments only.

➢ **Global measurements probe complementary properties**

Graphene with a twist





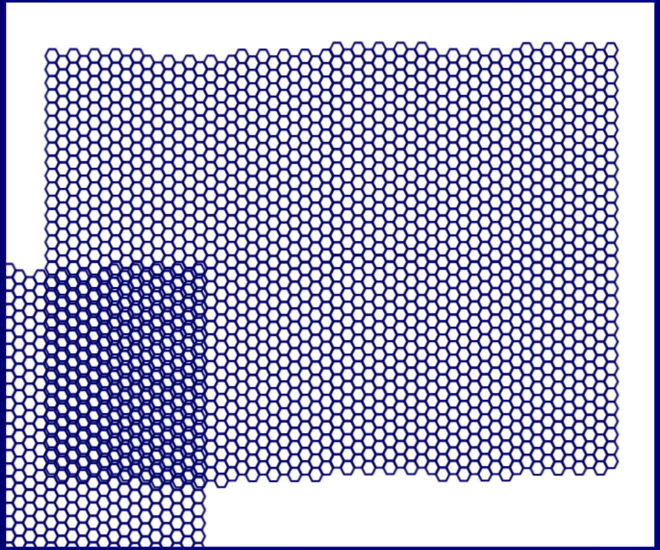


- Engineering electronic properties
  - Density of states
  - Landau levels in graphene
  - Scanning tunneling microscopy (STM) and spectroscopy (STS)
  - Atomic collapse and artificial atom
  - Kondo effect
  - Twisted graphene

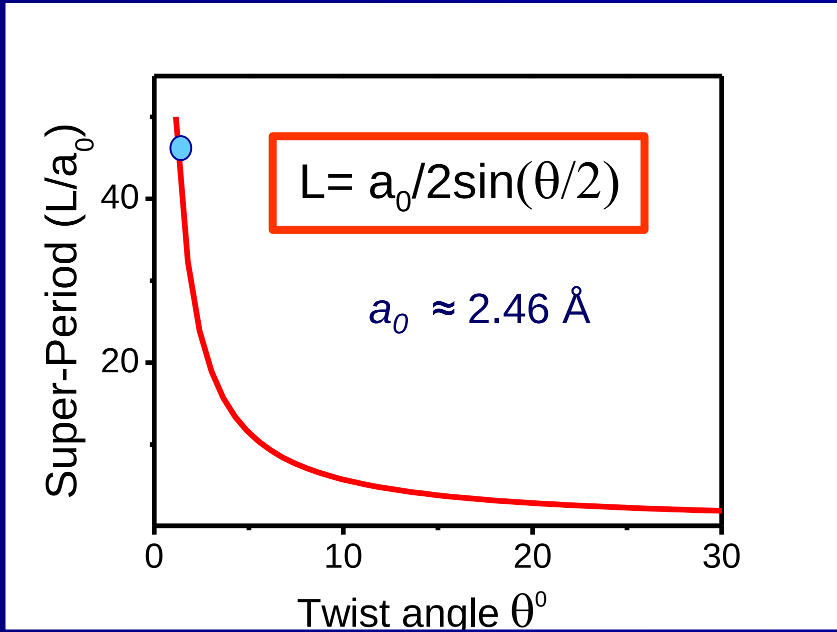
Twisted graphene – Moire patterns

Twist between layers $\mapsto$ Moiré pattern:

$\theta = 3^0$



Superstructure with period L



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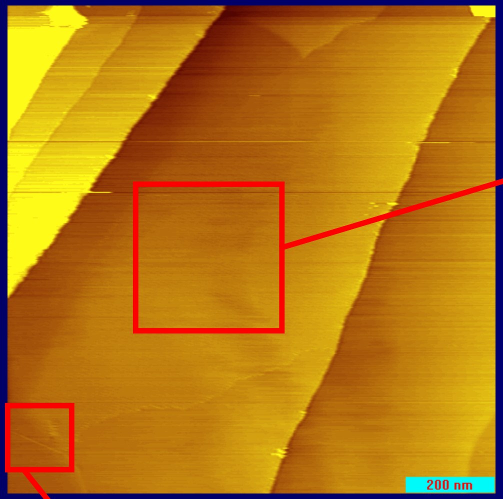
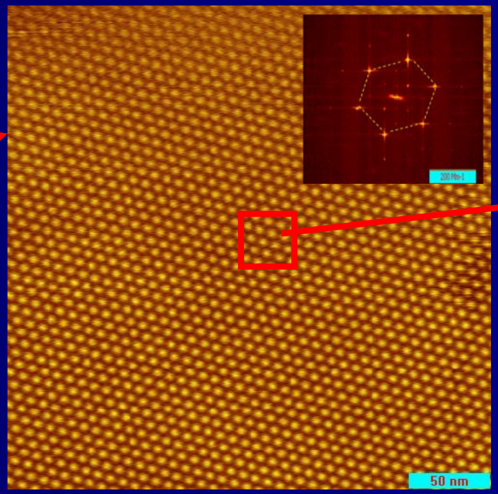
STM topography: Moiré superstructure

G. Li, et al Nature Physics (2010)

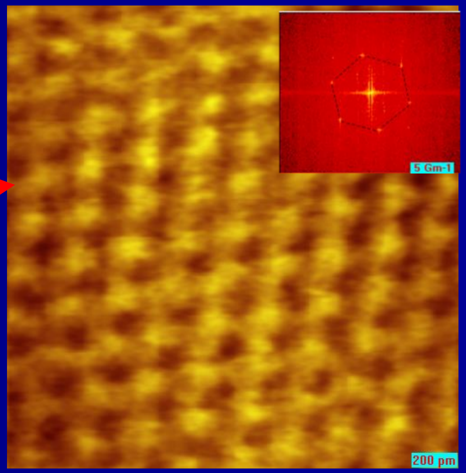
superstructure L=7.5nm → $\theta = 1.79^{o}$

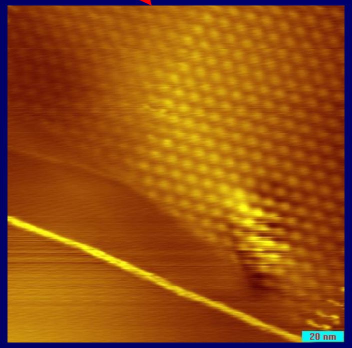


x4

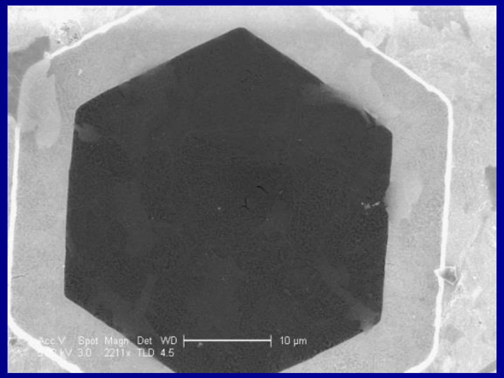


x250



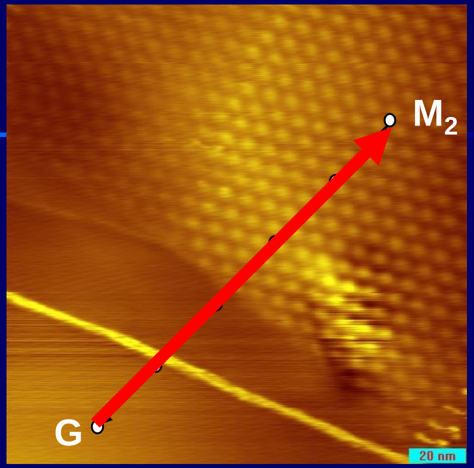


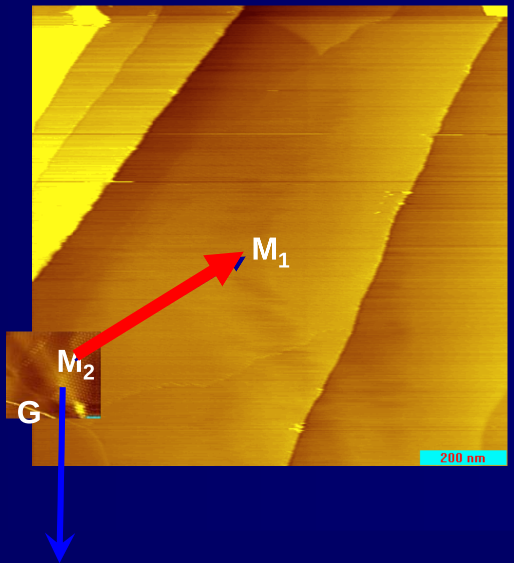
Boundary of area with superstructure

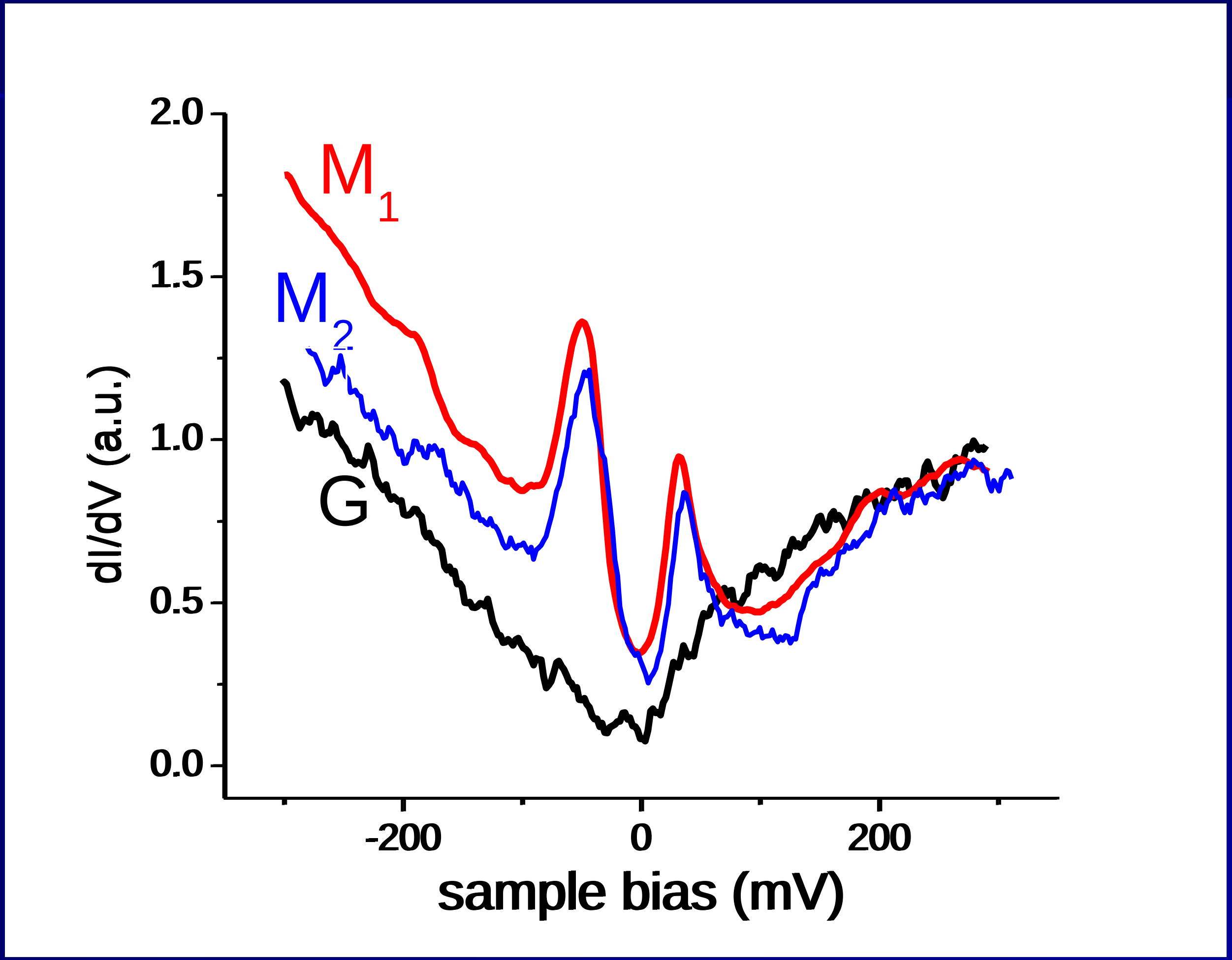


Spectroscopy Surprise

G. Li, et al Nature Physics (2010)







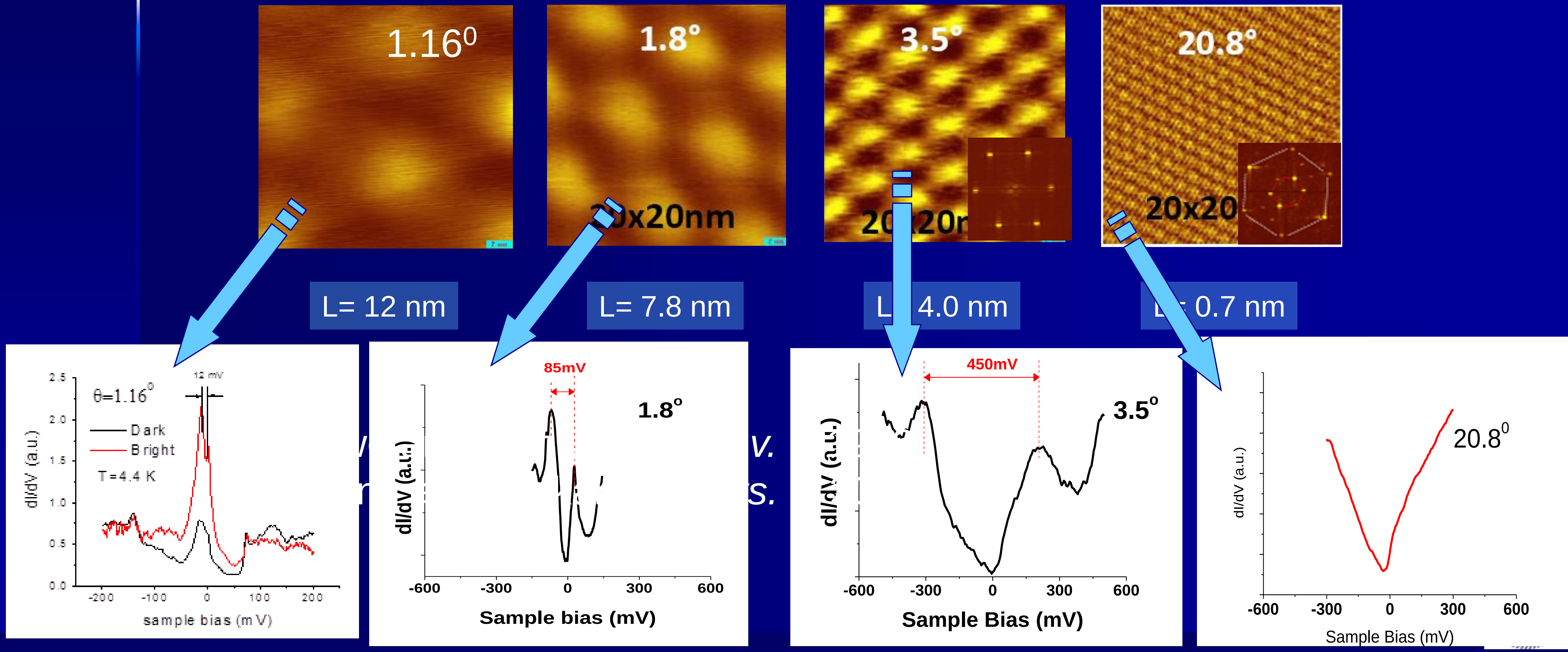
Two peak structure only in twisted region

E.Y. Andrei

Band structure of twisted graphene

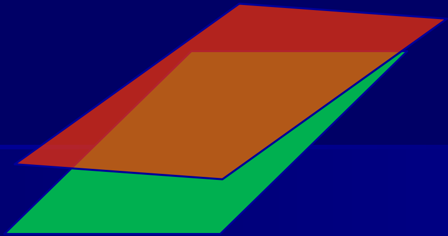
G. Li, *et al* Nature Physics **6**, 109 (2010)

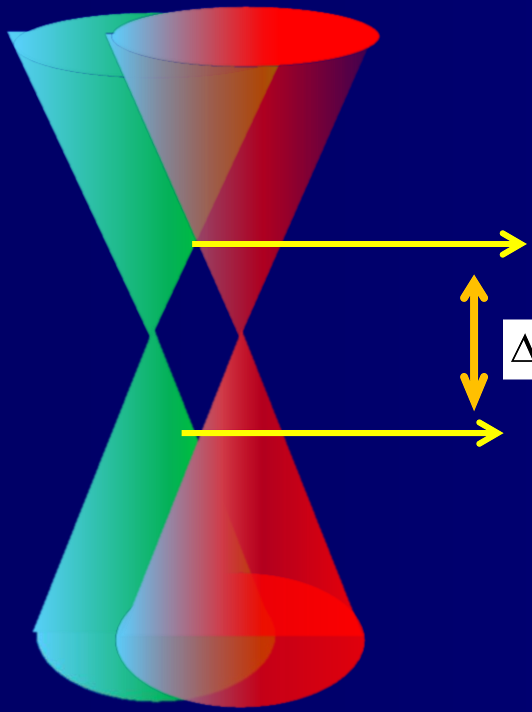
Increasing twist angle θ



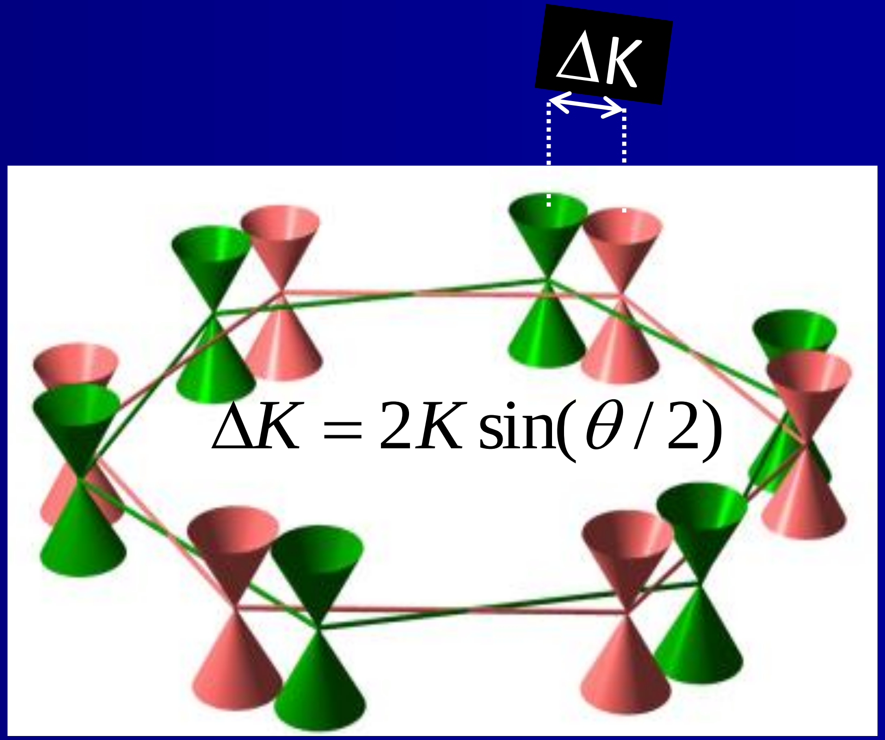
Band structure engineering with a twist

J. Lopes dos Santos, A.H. Castro Neto





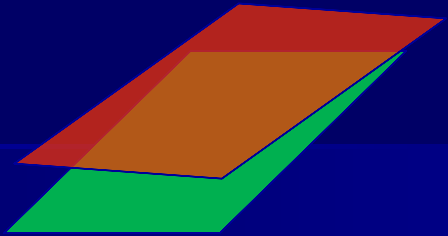
$$\Delta E = \hbar v_F \Delta K \propto sin(\theta/2)$$

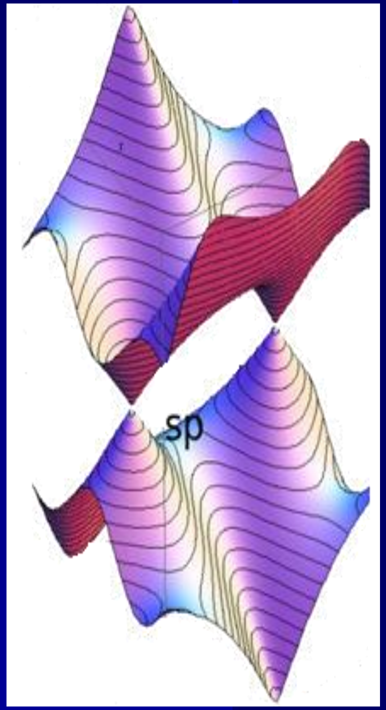


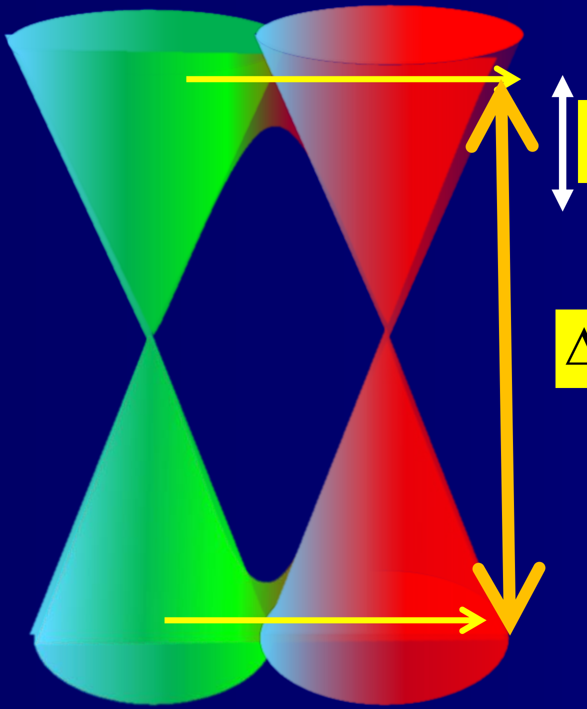
Band structure engineering with a twist

J. Lopes dos Santos, A.H. Castro Neto

Hybridization

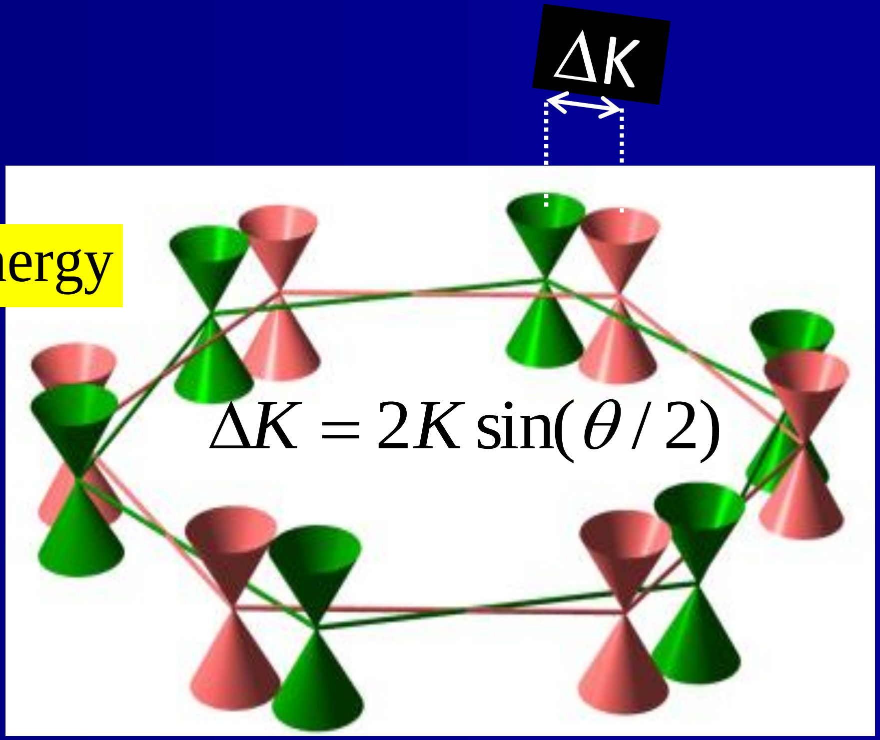






w hybridization energy

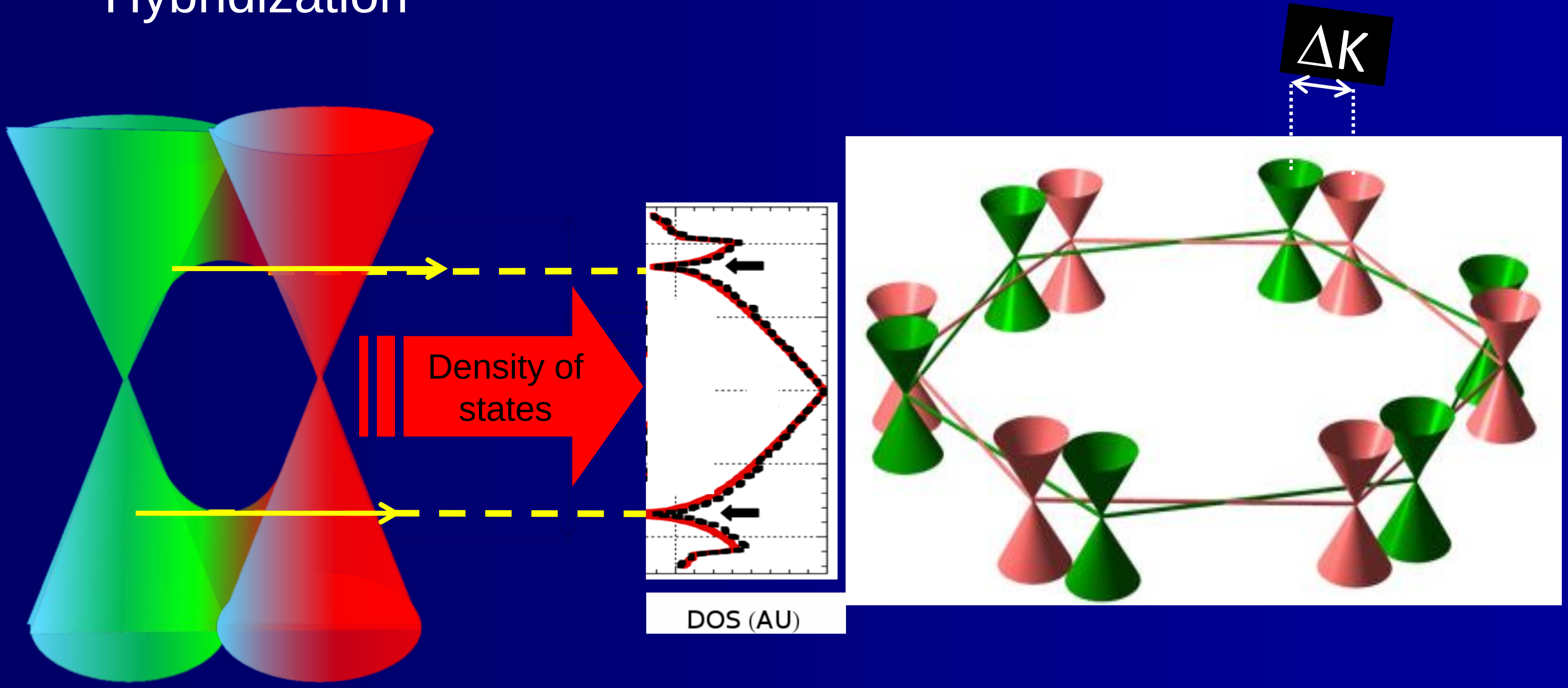
$\Delta E = \hbar v_F \Delta K - w$



Van Hove singularities

G. Li, et al Nature Physics (2010)
A. Luican, et al PRL 106, 126802 (2011)

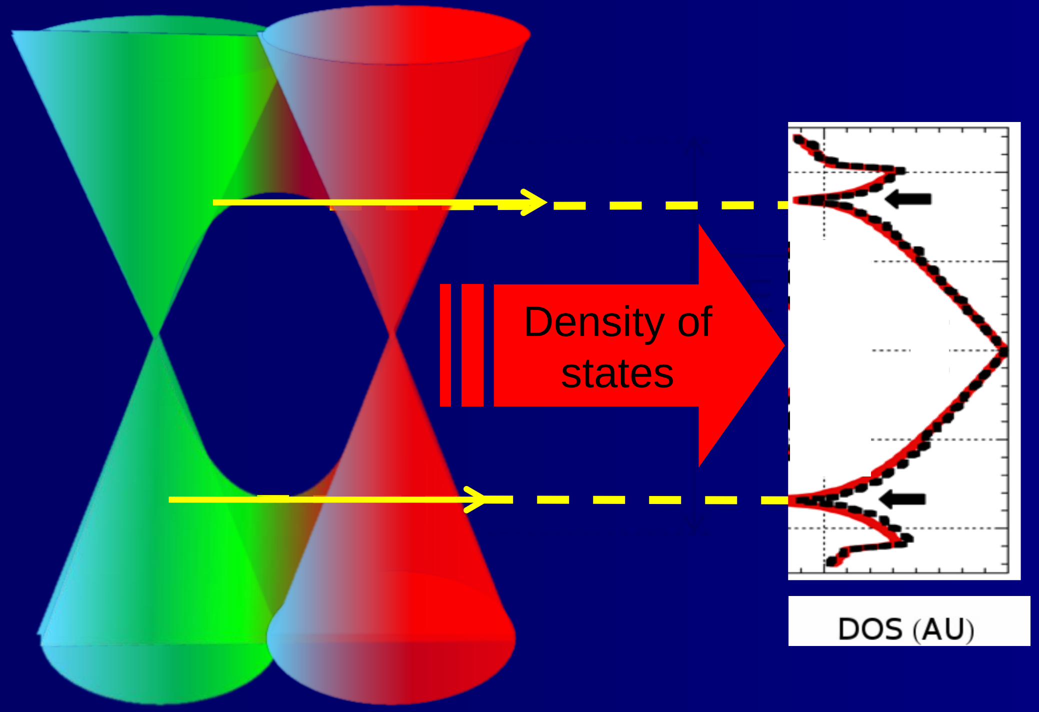
Hybridization



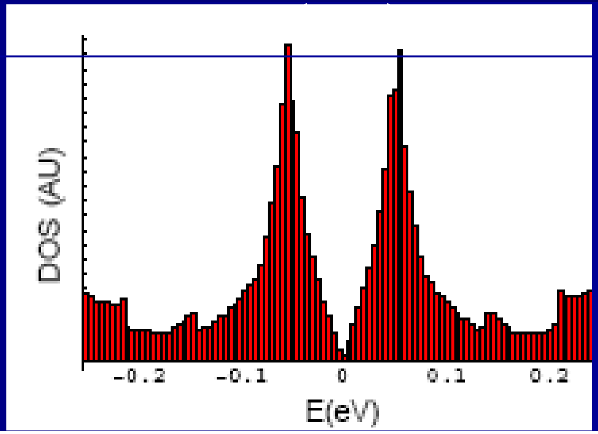
Twisted graphene
develops strong *Van Hove singularities*

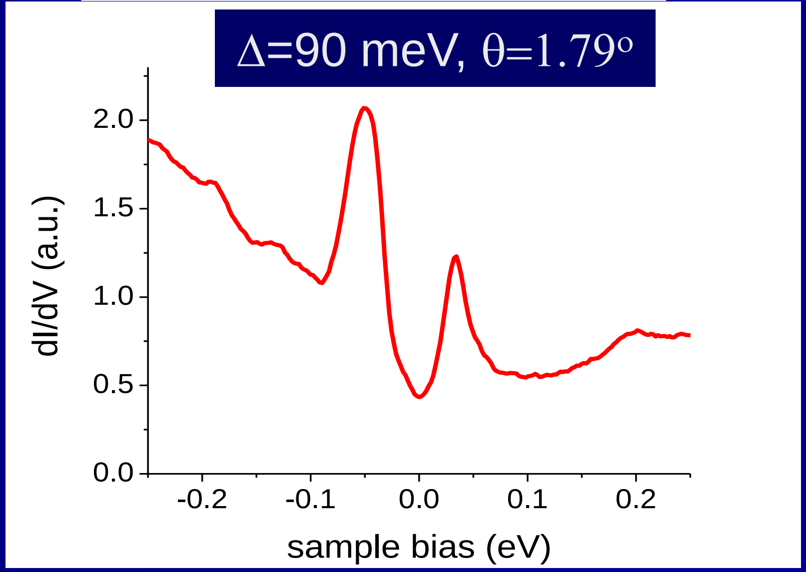
Van Hove singularities

G. Li, et al Nature Physics (2010)
A. Luican, et al PRL 106, 126802 (2011)



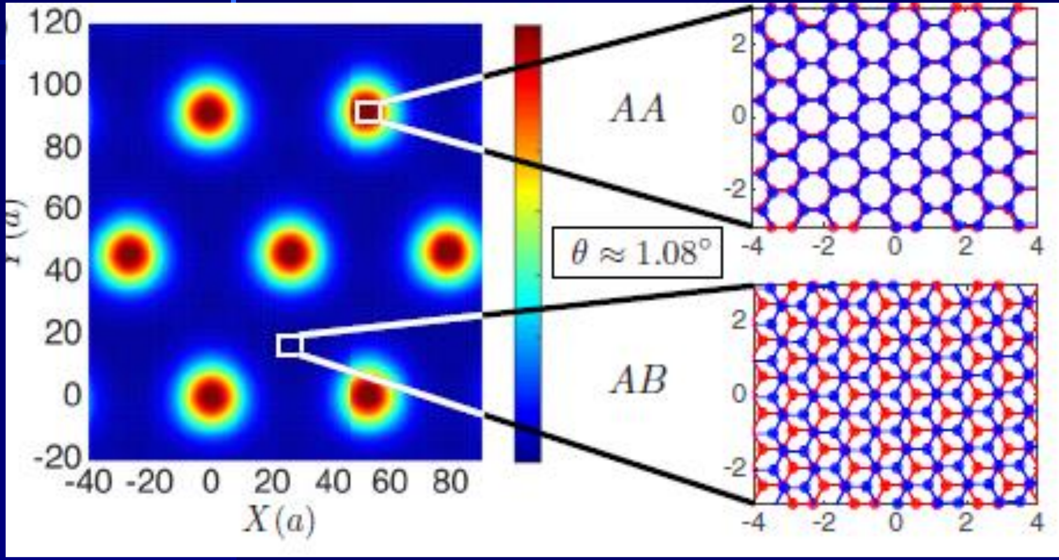
Low energy Band structure and DOS using perturbation theory





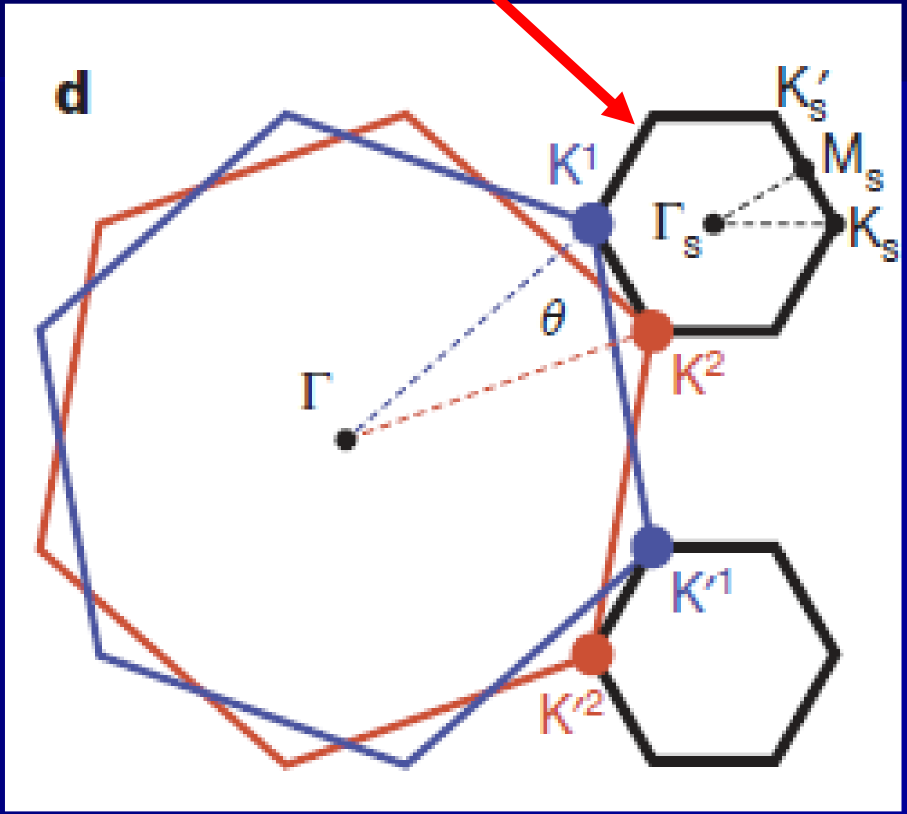
What happens at small twist angles?

DOS map

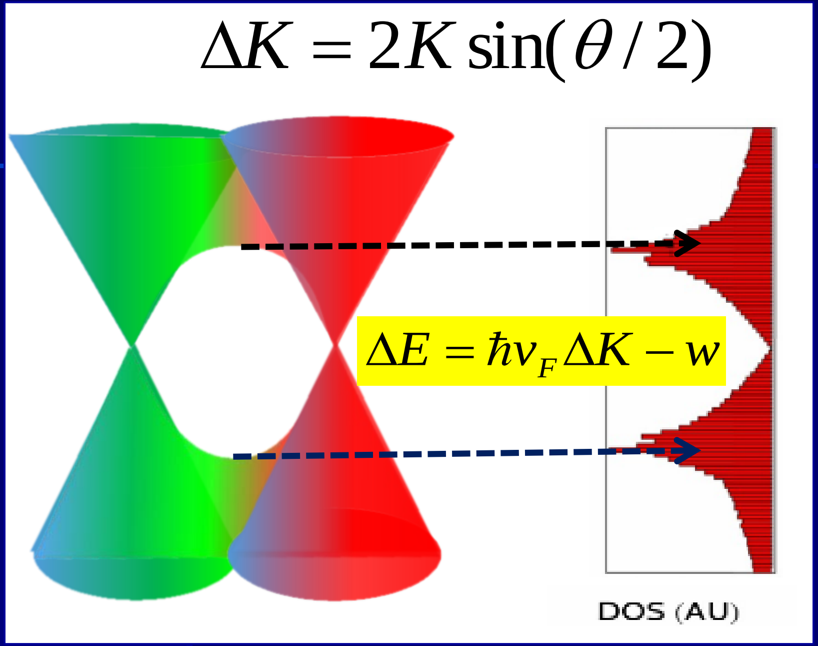


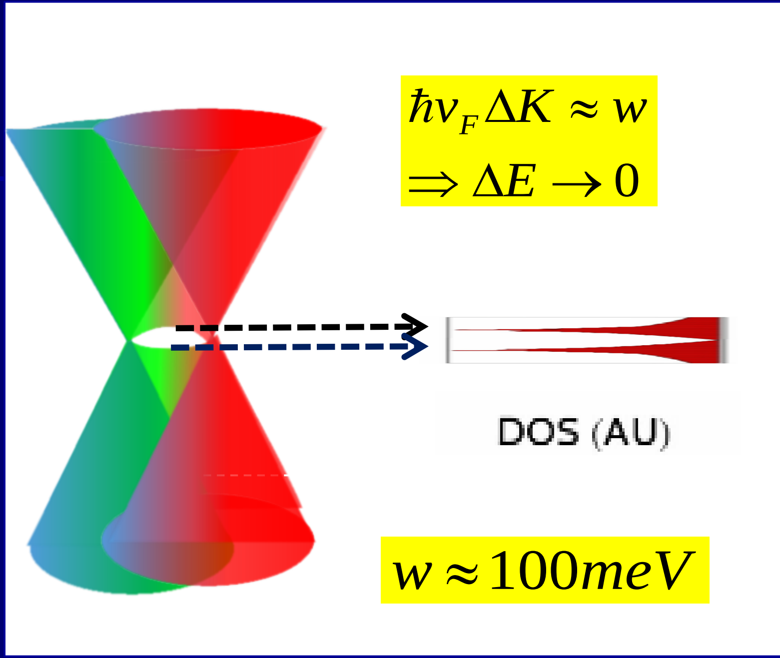
Moire units cell contains 1.3x10[4] atoms!

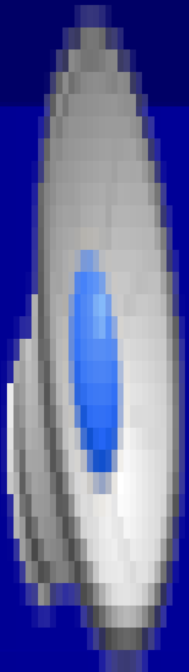
Moire Brillouin zone



What happens at small twist angles?







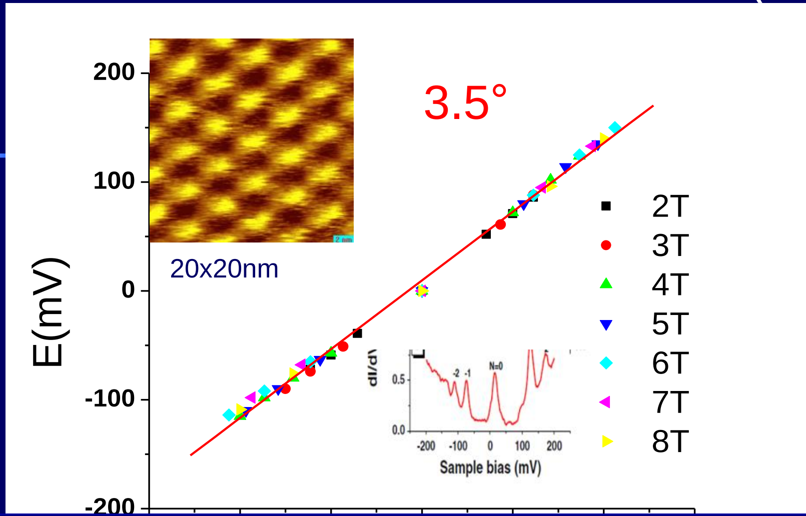
For $\hbar v_F \Delta K \approx w$ band flattens $\mapsto$ DOS diverges: Van Hove singularities.

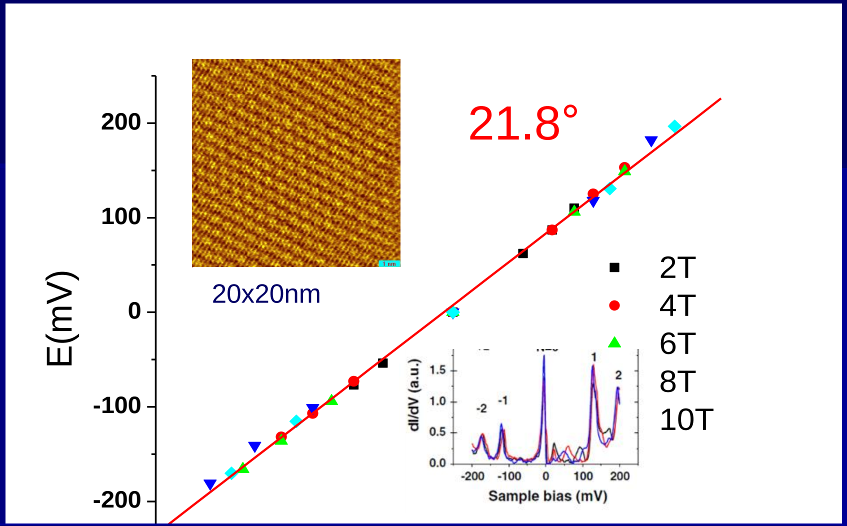
Magic angle: $\hbar v_F K \theta_M \approx w$

Using *w*~ 100meV $\theta_M \approx 1.09^0$

Fermi velocity : slowdown

A. Luican, et al PRL 106, 126802 (2011)

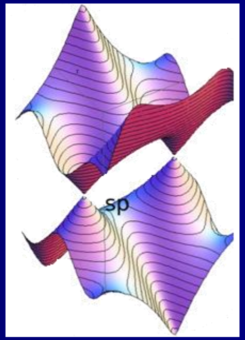


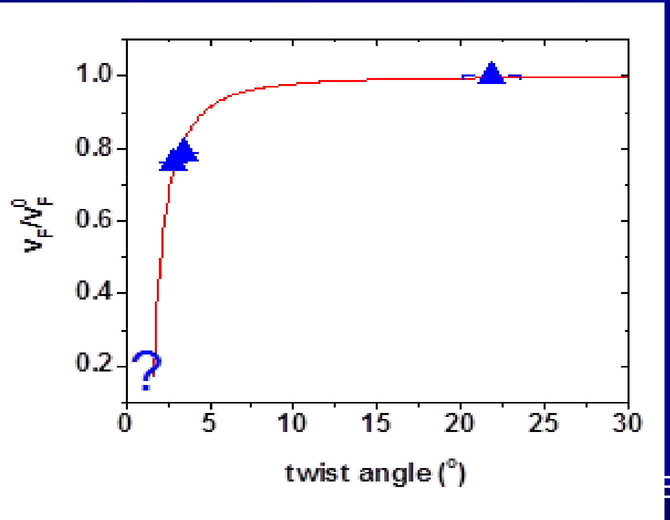


For $\theta > 10^0$

low energy band structure of twisted layers is identical to single layer

$$\frac{\tilde{v}_F(\theta)}{v_F} = 1 - 9\left(\frac{w}{\hbar v_F \Delta K}\right)^2$$





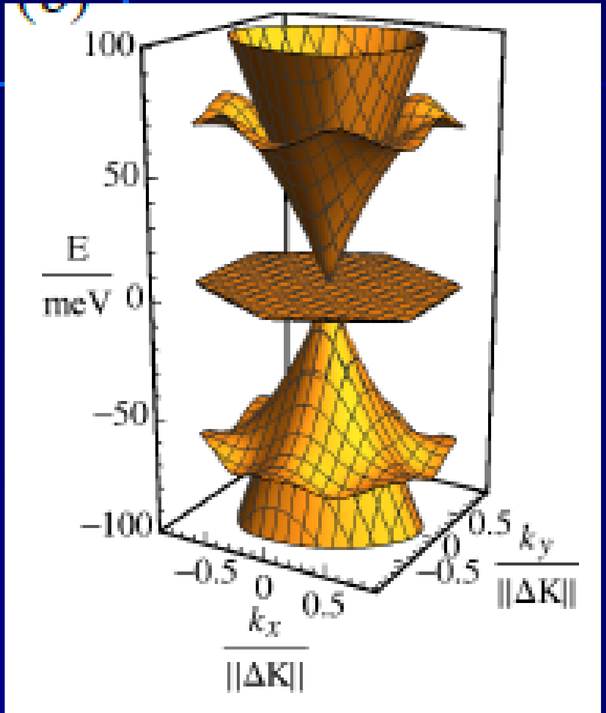
•J.M.B.L. dos Santos et al. PRL 99, 256802 (2007).

•G.T. Laissardière et al, Nanoletters ASAP (2009)

•Shallcross et al. PRL. 101, 056803 (2008)

•. R. Bistritzer, and A. H. MacDonald, (2010)

Correlation effects



- When the energy scale of electron-electron interactions is comparable to the band-width, correlation effects become important.
- At ½ filling (Fermi energy in middle of gap):

Correlated states can emerge: superconductivity, charge density waves, antiferromagnetism, topological insulators etc.

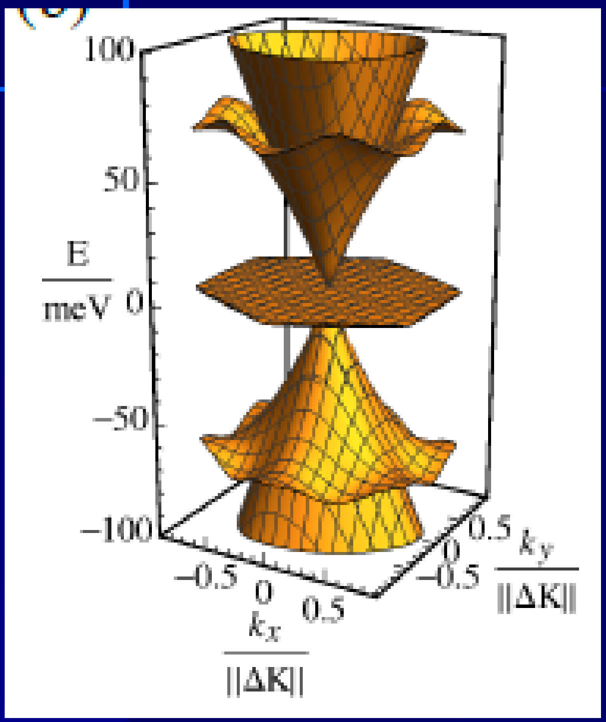
$$E_{coulomb} = \frac{e^2}{4\pi\varepsilon_0\kappa\lambda^2};$$

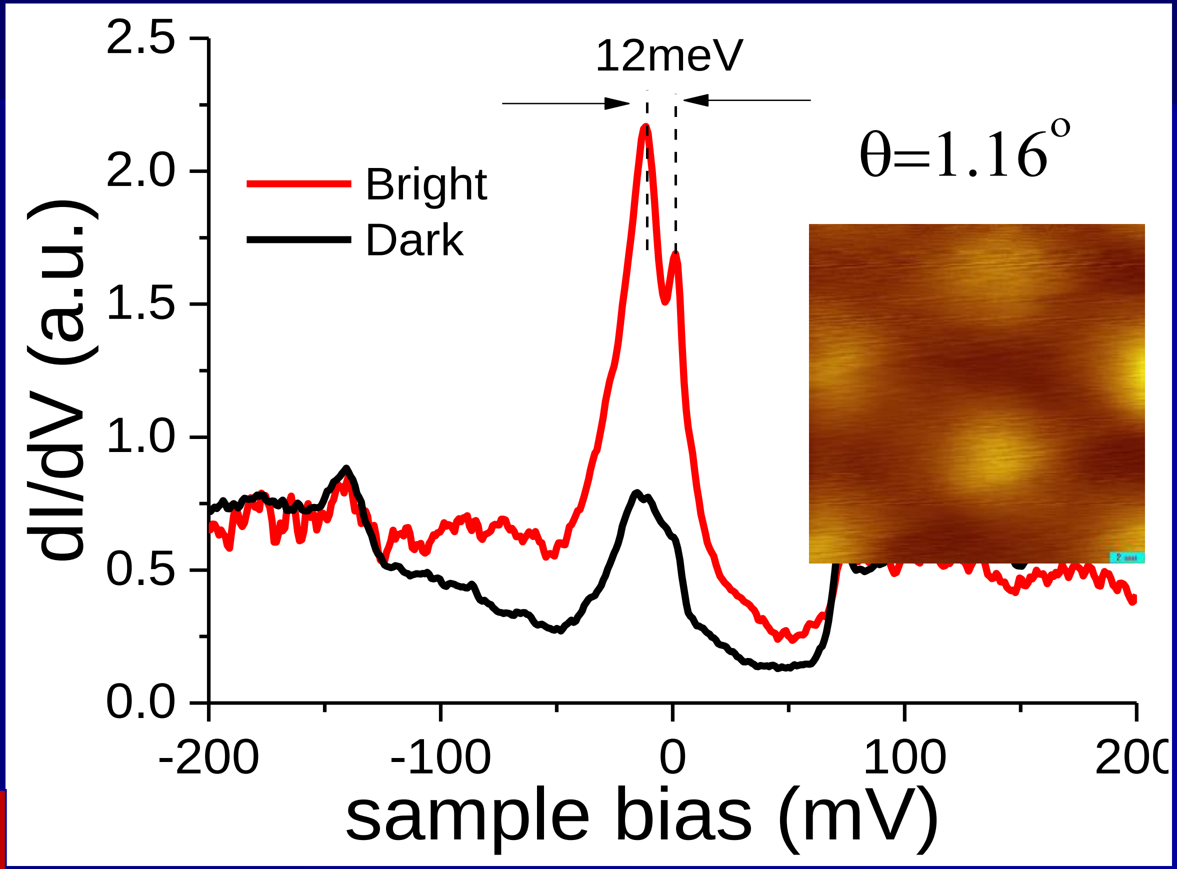
λ moire period;

κ dielectric constant

Correlation gap

G. Li, et al Nature Physics **6**, 109 (2010)





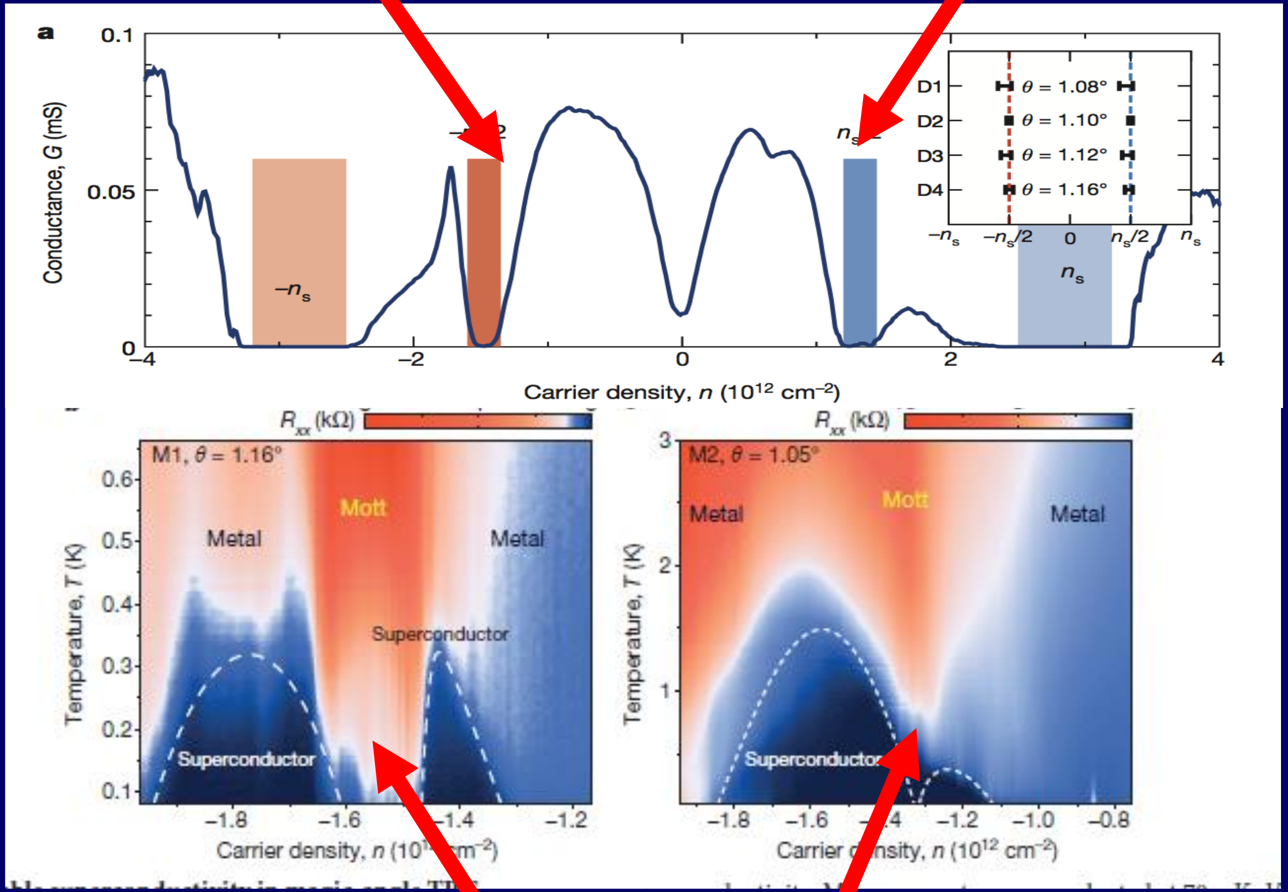
For $\theta = 1.16^0$

- 12meV Gap opens at the Fermi energy!
- Correlation gap – CDW?

2018 –Magic angle insulator and superconductor

Y. Cao et al., Nature(2018)

- Half Full band – 2 electrons (holes) per moire cell.



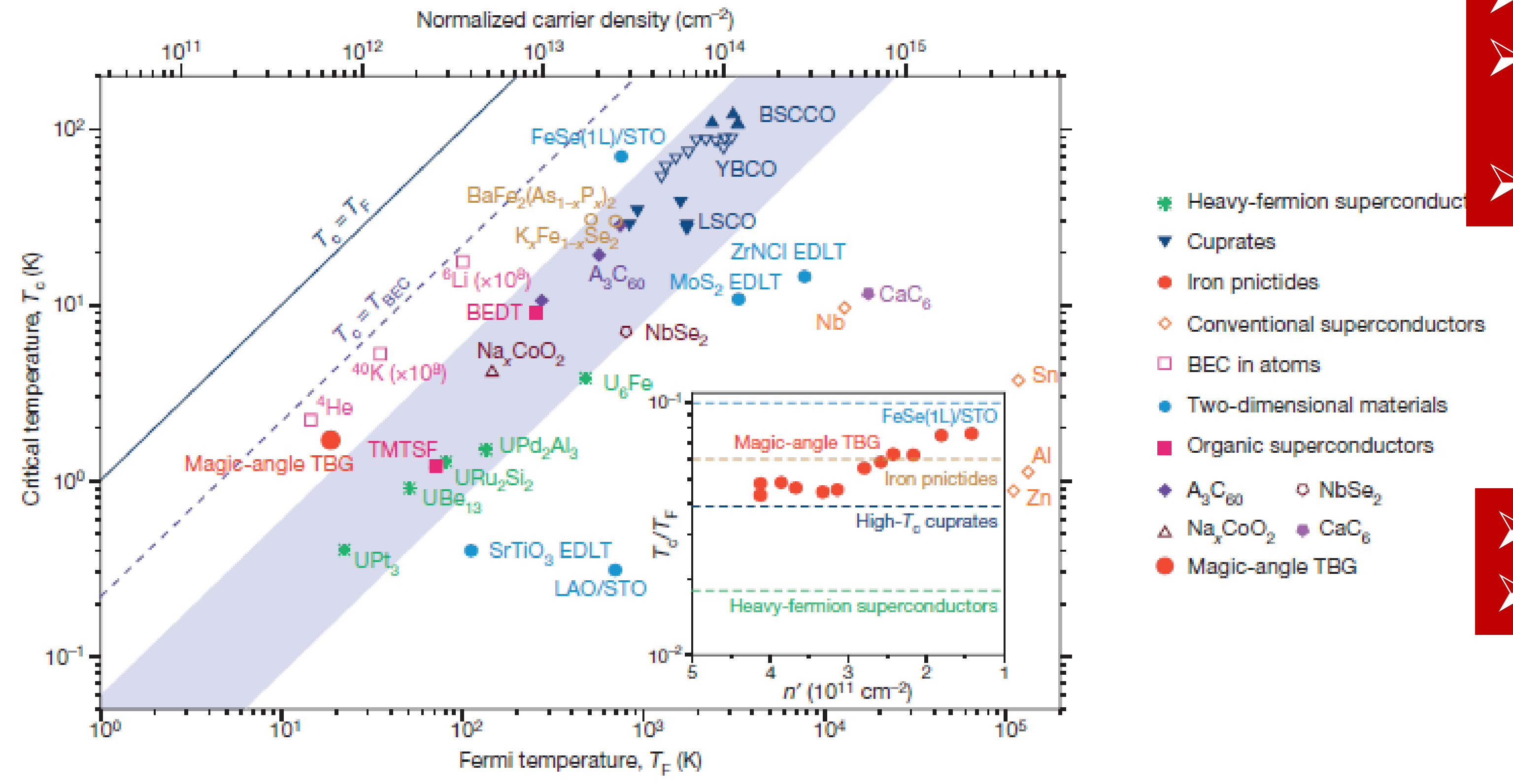
- ½ Full band – insulating phase ~ 4K
- Insulating phase flanked by 2 superconducting domes slightly off half-filling
- Maximum Tc ~1.7K
- $T_c/E_F \sim 10^{-1} \mapsto$ strong coupling

- Resembles high Tc superconductors
- BUT tunable doping and Tc

½ Full band – 2 electrons (holes) per moire cell.

Strongly coupled superconductor

Y. Cao et al., Nature(2018)



- ½ Full band – insulating phase ~ 4K
- Insulating phase flanked by 2 superconducting domes
- $T_c/E_F \sim 10^{-1} \mapsto$ strong coupling

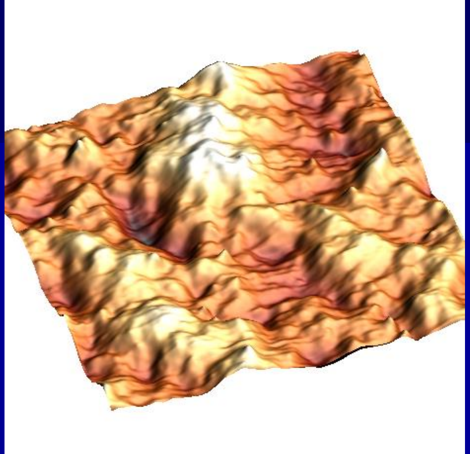
- Resembles high Tc superconductors
- BUT tunable doping and Tc

OPEN QUESTIONS:

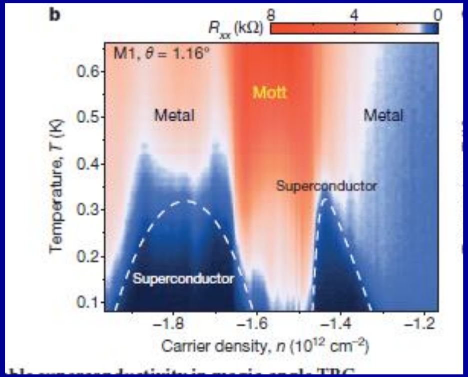
- Pairing mechanism
- Gap symmetry
- Nature of insulating phase

Summary of part IV

- Kondo screening in graphene occurs above a critical coupling strength
- Magnetic moments in graphene can be tuned with gating or local curvature
- If coupling strength is non-uniform global measurements are misleading



- Band structure of bilayer graphene can be tuned with twist angle
- At small twist angles the DOS develops Van-Hove singularities
- At the "magic angle" $\theta \sim 1.1^0$ a flat band forms at the charge neutrality point
- At half filling the flat band developconductings strong correlations resulting in an insulating phase flanked by superconducting domes.



2D materials are cool!