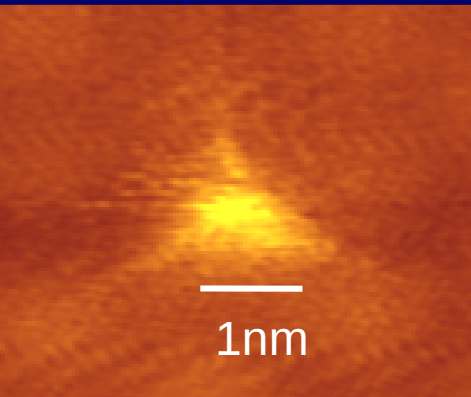
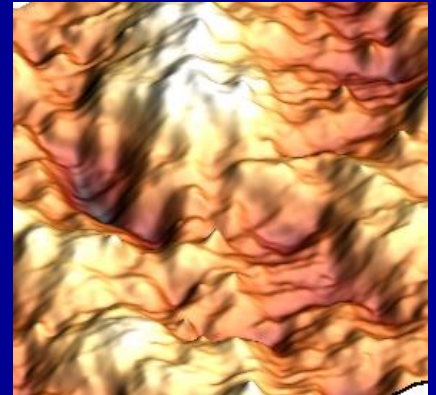


# Kondo Screening of Moments in Imperfect Graphene

- Vacancy magnetic moment
- Kondo screening of magnetic moments
- Gate tunable magnetic moment
- Screening on a curved surface



*Eva Y. Andrei*  
*Rutgers University*



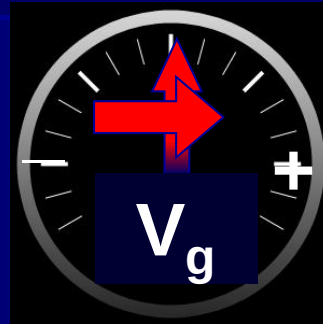
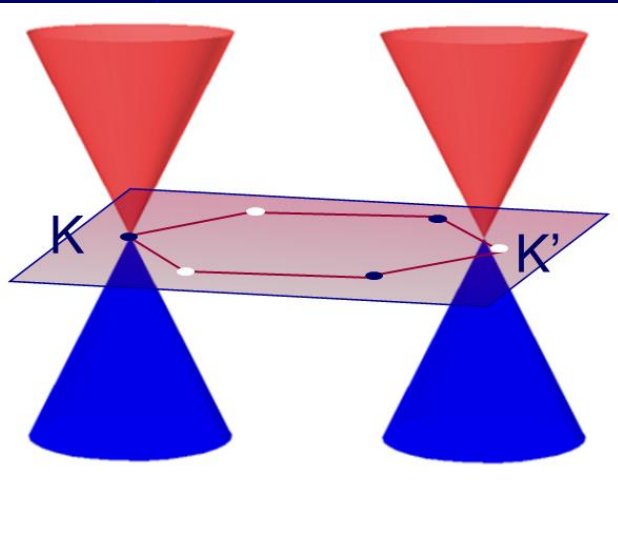
118th Statistical Mechanics Conference Rutgers Dec 2017

*Honoring: Guenther, Cristina and Shelly*



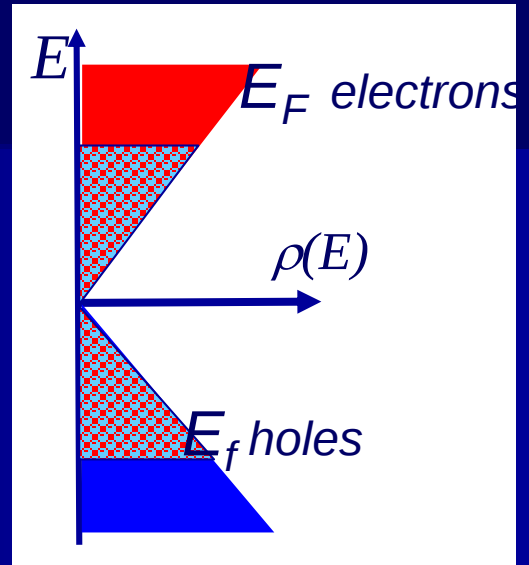
# Perfect Graphene

## Band structure



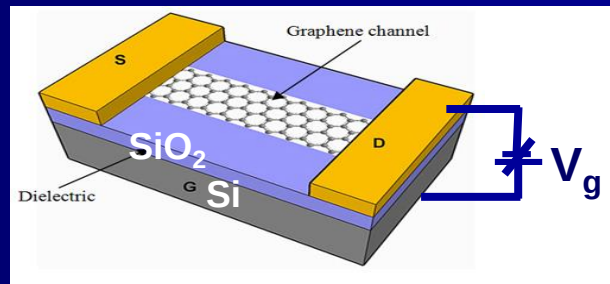
$$1\text{V} \mapsto 7 \times 10^{10} \text{ cm}^{-2}$$

## Density of states



## Ingredients:

1. 2D
2. Honeycomb structure ● ●
3. Identical atoms



# Magnetism and Perfect Graphene



VOLUME 62, NUMBER 10

PHYSICAL REVIEW LETTERS

6 MARCH 1989

## Two Theorems on the Hubbard Model

Elliott H. Lieb

*Departments of Physics and Mathematics, Princeton University, P. O. Box 708, Princeton, New Jersey 08544*  
(Received 12 December 1988)

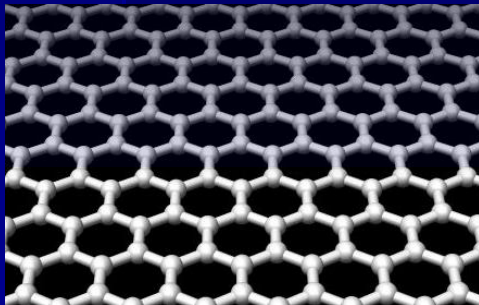
In the attractive Hubbard model (and some extended versions of it), the ground state is proved to have spin angular momentum  $S=0$  for every (even) electron filling. In the repulsive case, and with a bipartite lattice and a half-filled band, the ground state has  $S = \frac{1}{2} |B| - |A|$ , where  $|B|$  ( $|A|$ ) is the number of sites in the  $B$  ( $A$ ) sublattice. In both cases the ground state is unique. The second theorem confirms an old, unproved conjecture in the  $|B| = |A|$  case and yields, with  $|B| \neq |A|$ , the first provable example of itinerant-electron ferromagnetism. The theorems hold in all dimensions without even the necessity of a periodic lattice structure.

...repulsive Hubbard with **bipartite lattice** and **half-filled** band:

➤ spin of ground state with  $N_A, N_B$  populated sites:

$$S = \frac{1}{2}(N_A - N_B)$$

Pristine graphene (graphite)  $N_A = N_B \rightarrow S = 0$



Perfect graphene  
Non-Magnetic!

- T. L. Makarova, et al *Nature* 413, 716 (2001) (RT ferromagnetism in C60)
- D. P. Esquinazi, et al *Phys. Rev. B* (2002). (Ferromagnetism in graphite)
- R. A. Wood, et al *J. Phys. Condens. Matter* (2002) (Ferromagnetic fullerenes)
- J. M. D. Coey et al, *Nature* 420, 156 (2002). (Extra-terrestrial graphite)

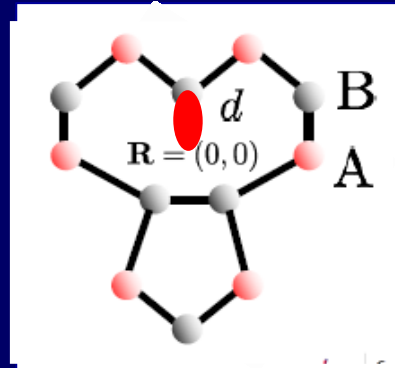
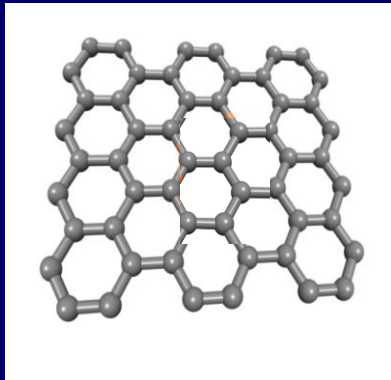
Vacancies in graphene  $\rightarrow N_A > N_B \rightarrow$  magnetic moment  $> 1\mu_B$

A.H. Castro Neto et al. *Solid State Commun.* (2009).  
T. Wehling, *Phys. Lett.* (2009)  
O. Yazyev, et al *Rep. Prog.* (2010).  
M. Vojta et al, *EPL*, 90 (2010) 27006  
T. O. Wehling, *Phys. Rev. B* 81, 115427(2010)  
J. O. Sofo, et al *Phys. Rev. B* 85, 115405 (2012)

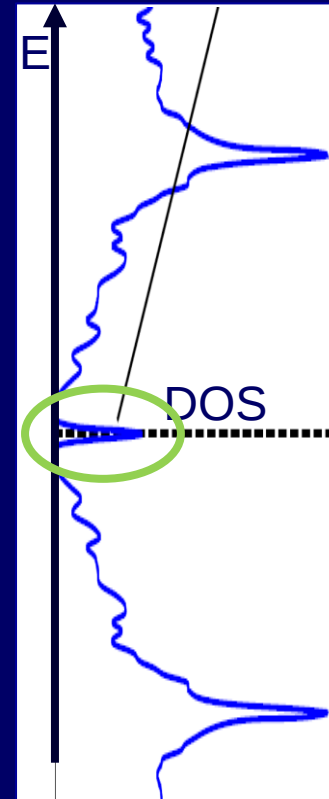
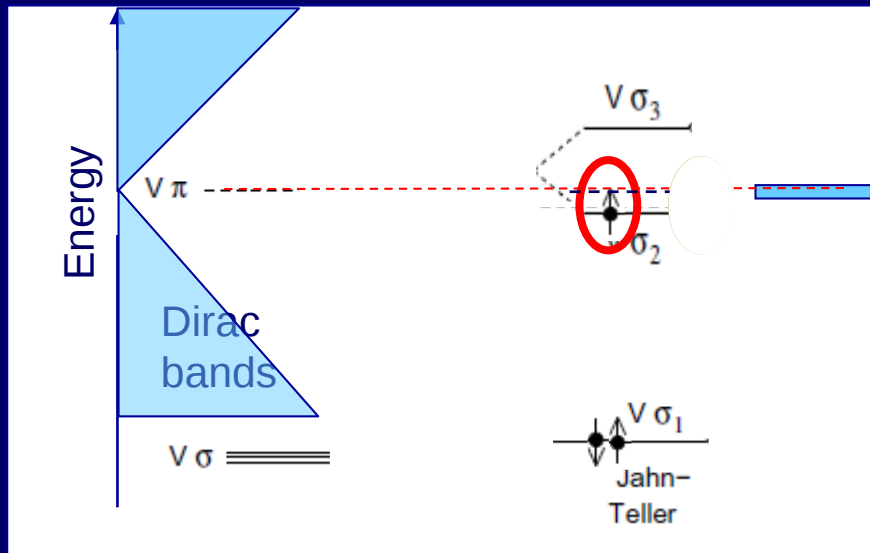
E.Y. Andrei



# Imperfect Graphene - Vacancy



Yazyev & Helm (2007),  
Popovi'c, Nanda, Satpathy (2012)



Broken  
AB  
symmetry

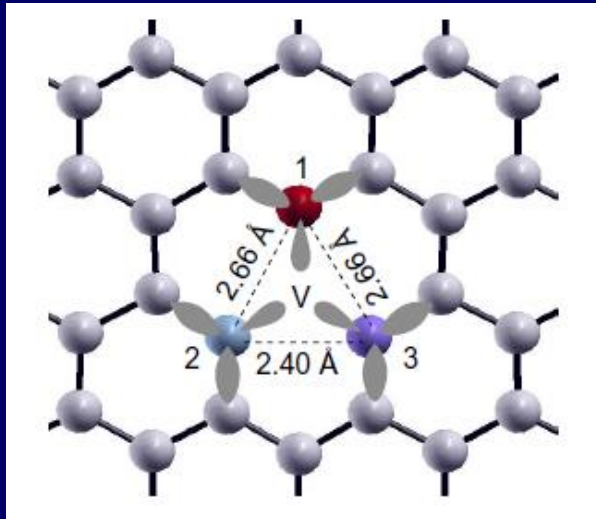
$\sigma$  Dangling bond  $\mapsto$  localized state  $\mapsto 1\mu_B$

$p_z$   $\mapsto$  quasi-localized state on other sublattice  $\mapsto \sim 0.5-0.7\mu_B$

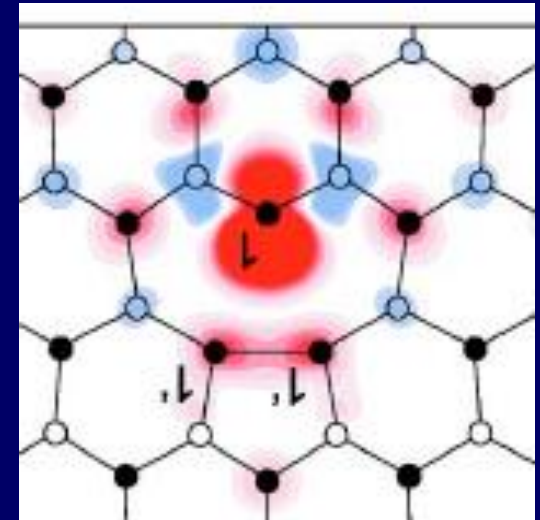
Zero mode peak at  $\sim$ Dirac Point



# Imperfect Graphene - Vacancy



Magnetic Moment



Magnetic moment  $\sim 1.7\mu_B$

Yazyev & Helm (2007)

Interaction of ultra-relativistic electrons with Local magnetic moment?

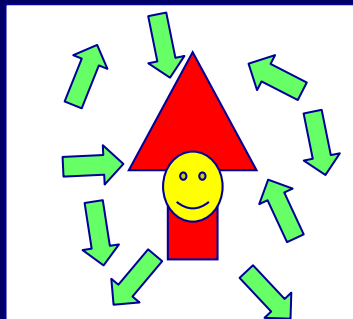




# Kondo Screening of Impurity Moments in Metals

$T > T_K$

Unscreened

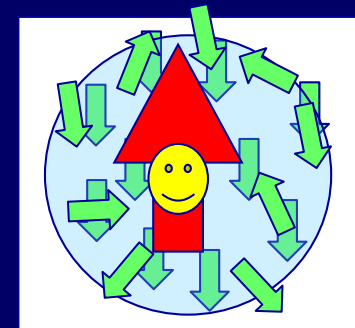


Impurity spin in metal

$J$  antiferromagnetic  
coupling to electron bath

$T < T_K$

Screened



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

$\rho$  density of states at  $E_F$

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

❖ Normal metals  $\rho(E_F) \sim \text{finite}; J \neq 0 \rightarrow T_K > 0$

❖ Insulators  $\rho(E_F) = 0$  No Kondo screening

What happens in a pseudogap system?



# Kondo Screening in pseudo-gap systems

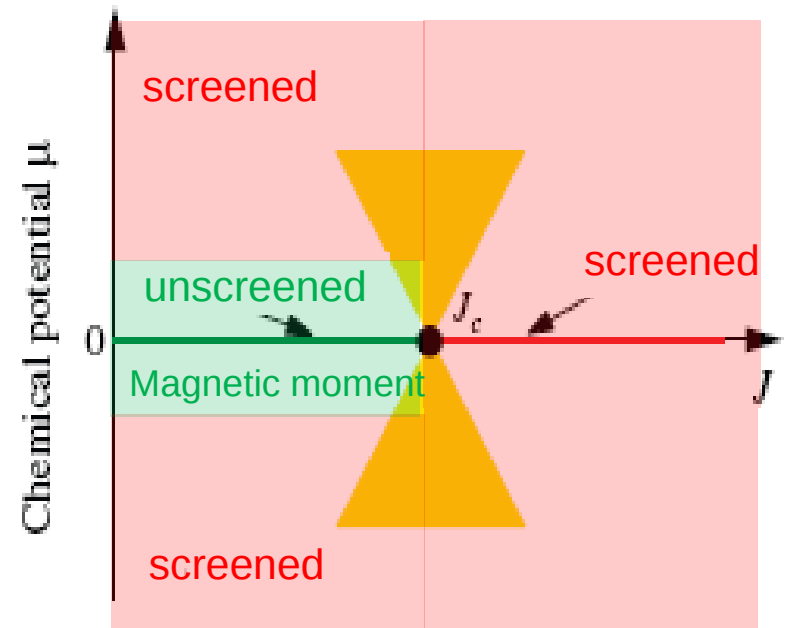
- Pseudo-gap systems  $\rho(E) \propto E^r$  screening suppressed.
- ❖  $r = 1$  (graphene, high  $T_c$  superconductors)

$\mu \sim 0$  (undoped)

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

$|\mu| \gg 0$  doped

- Normal Kondo screening



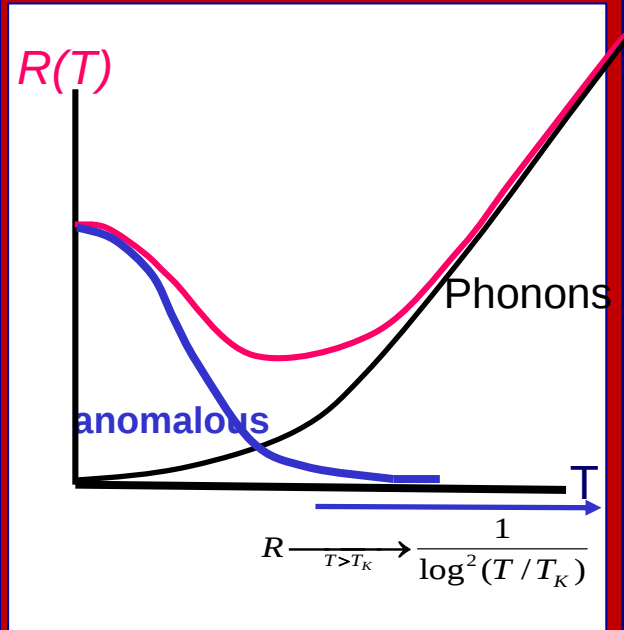
- D. Withoff and E. Fradkin, Phys. Rev. Lett. 64, 1835(1990)
- K. Chen and C. Jayaprakash, J. Phys L491 (1995)
- K. Ingersent, Phys. Rev. B54, 11936 (1996)
- C. Cassanello and E. Fradkin, (1996)
- R. Bulla, T. Pruschke, and A. C. Hewson, (1998)
- Polkovnikov A., Phys. Rev. B, 65 (2002) 064503
- Vojta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



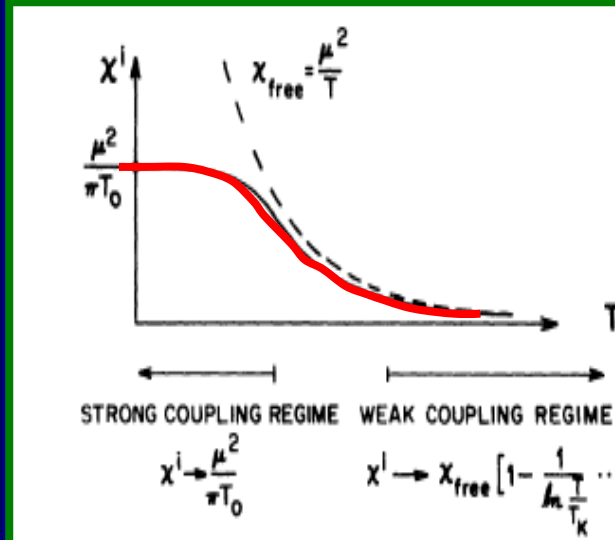


# Kondo Screening Experimental Signatures

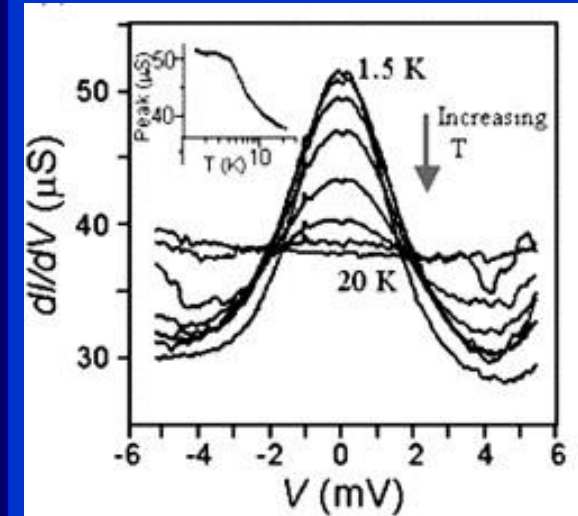
## Resistance minimum



## Magnetization saturation



## DOS – Kondo Peak



- Kondo Peak at  $E_F$
- Appears at  $T \sim T_K$
- Low T linewidth  $\Gamma$

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

DOS enhancement at  $E_F$

nature physics

LETTER

PUBLISHED ONLINE: 3 APRIL 2011 | DOI: 10.1038/NPHYS121

**Tunable Kondo effect in graphene with defects**

Jian-Hao Chen<sup>1,2†</sup>, Liang Li<sup>2</sup>, William G. Cullen<sup>1,2</sup>, Ellen D. Williams<sup>1,2</sup> and Michael S. Fuhrer<sup>1,2\*</sup>

nature physics

LETTERS

PUBLISHED ONLINE: 10 JANUARY 2012 | DOI: 10.1038/NPHYS218

**Spin-half paramagnetism in graphene induced by point defects**

R. R. Nair<sup>1</sup>, M. Sepioni<sup>1</sup>, I-Ling Tsai<sup>1</sup>, O. Lehtinen<sup>2</sup>, J. Keinonen<sup>2</sup>, A. V. Krashenninnikov<sup>2,3</sup>, T. Thomsen<sup>4</sup>, A. K. Geim<sup>1</sup> and I. V. Grigorieva<sup>1\*</sup>

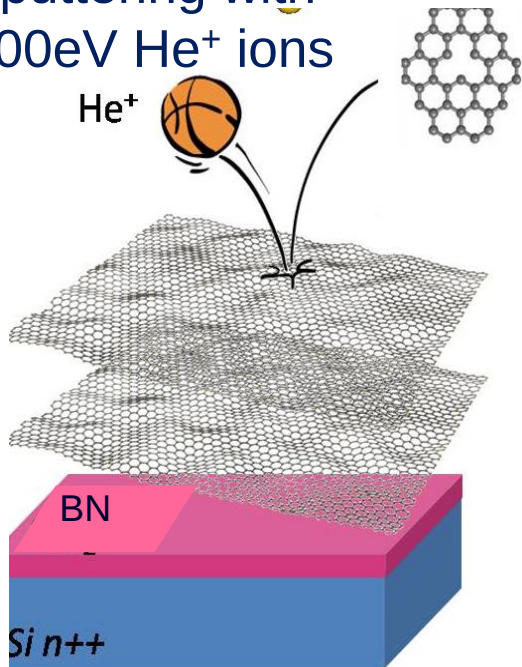
Measures:  
Unscreened moment

Measures:  
scattering off Kondo cloud

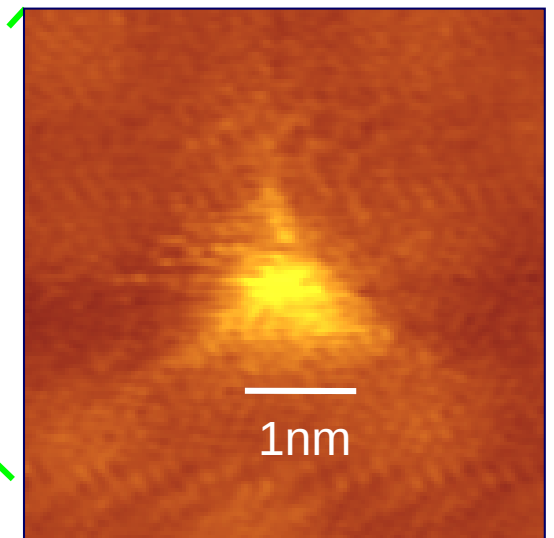
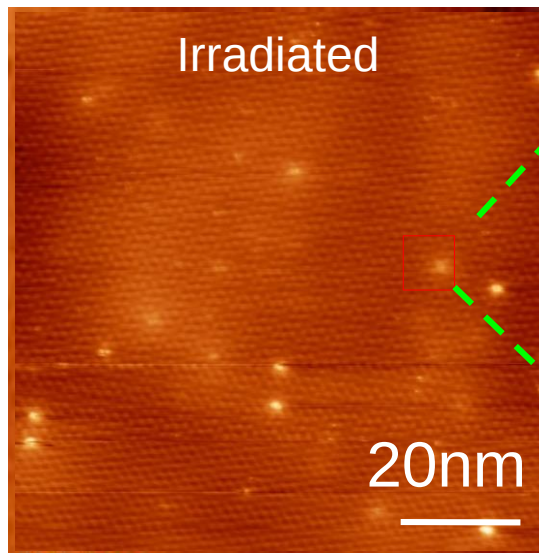


# Creating Vacancies

Sputtering with  
100eV  $\text{He}^+$  ions



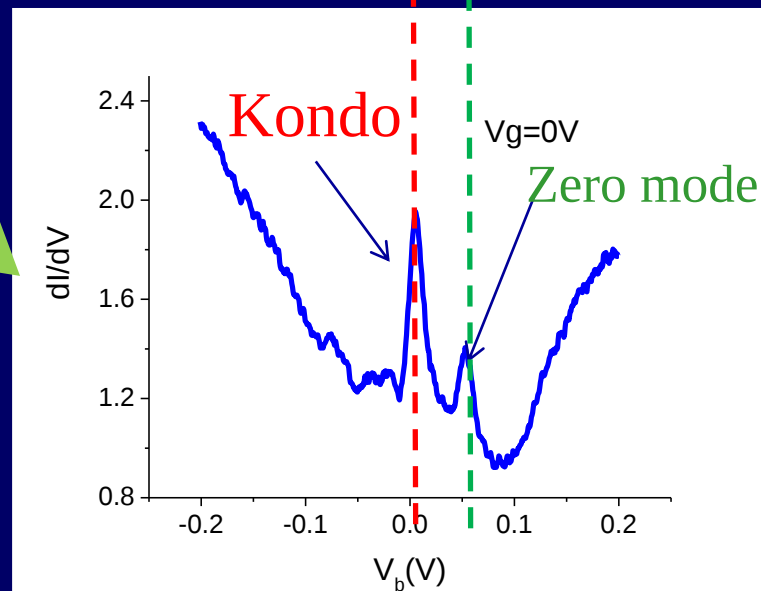
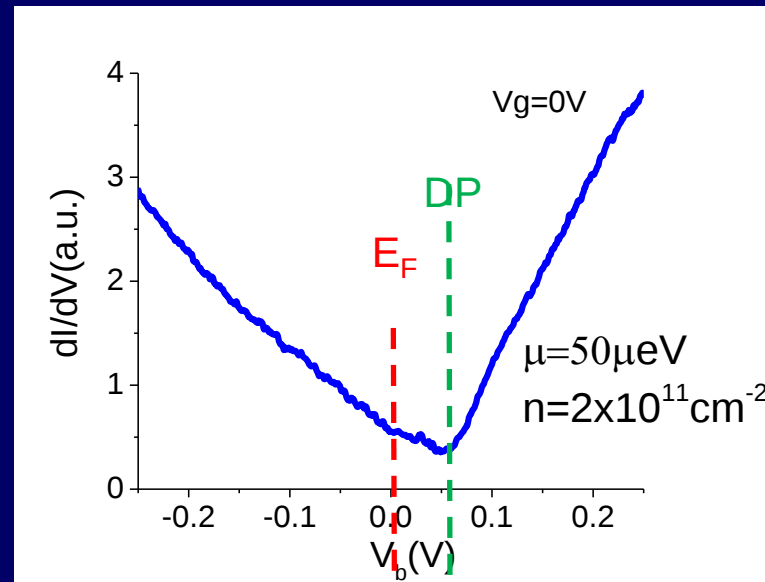
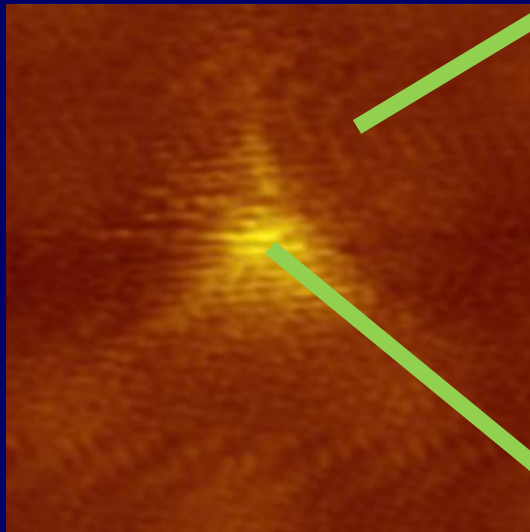
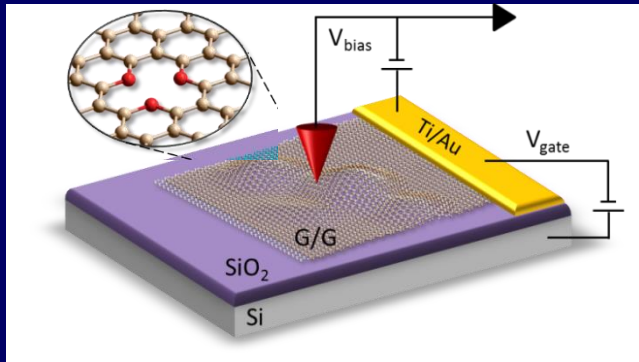
STM Topography



Single atom vacancy  $\rightarrow$  triangular structure.



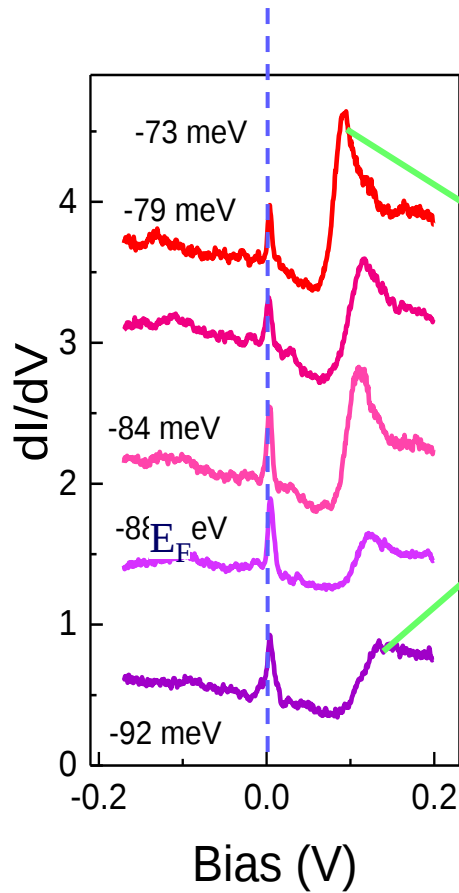
# STS: DOS Peak at $E_F$



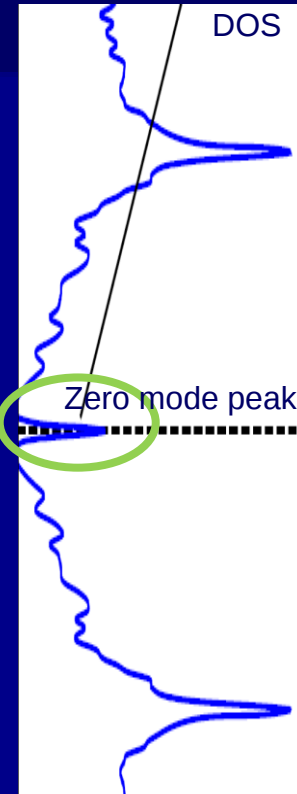
# Gate Dependence

Increasing  $\mu$

Kondo peak



Zero mode



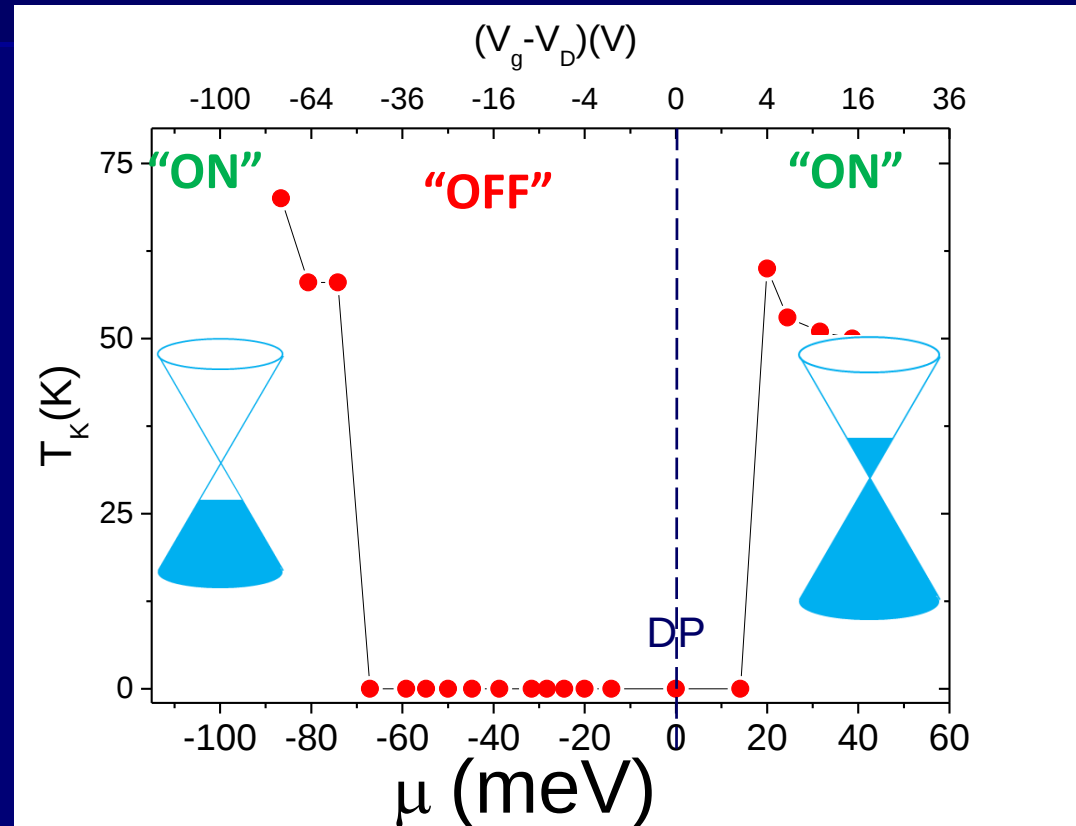
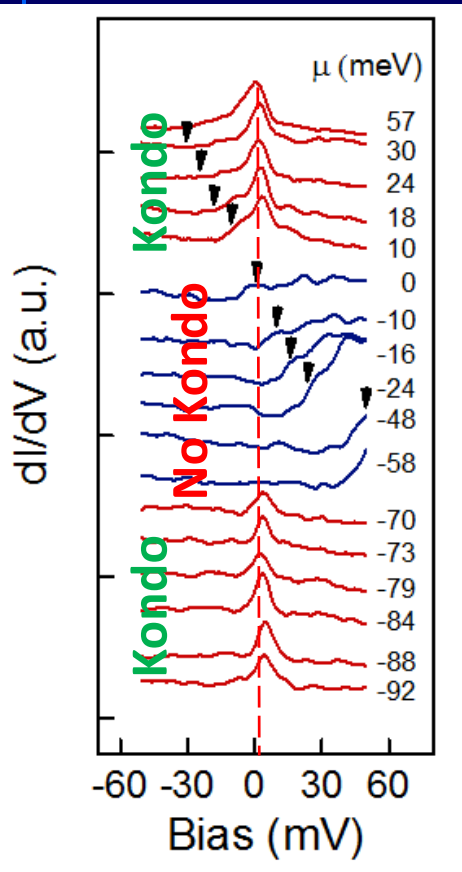
Pinned to  $E_F$



# Reentrant Kondo Screening

$$J < J_c$$

Increasing  $\mu$

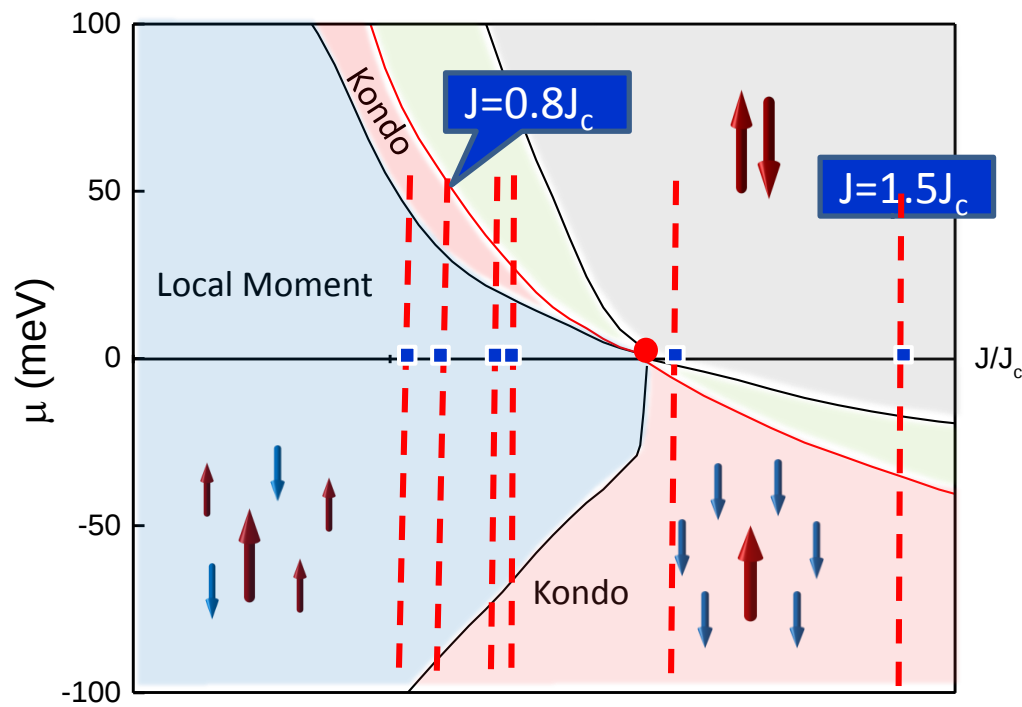


*Electrically tunable magnetic moment*



# Kondo Screening Phase Diagram

## Numerical Renormalization Group

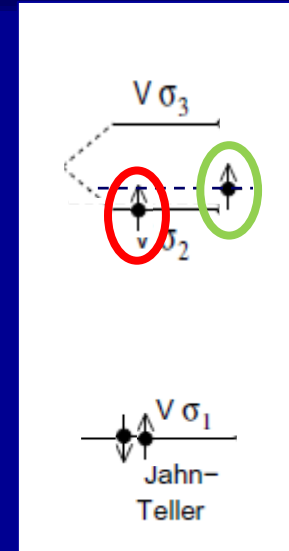
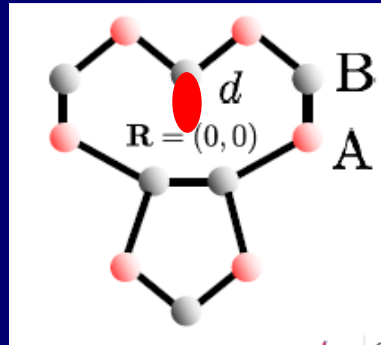


P.W Lo, GY Guo, F. Anders



# What is the value of $J$ ?

- $\sigma$  Dangling bond  $\mapsto$  localized state  $\mapsto 1\mu_B$
- $p_z$   $\mapsto$  quasi-localized state on other sublattice  $\mapsto \sim 0.5-0.7\mu_B$



➤  $\sigma$  state (in plane) – **orthogonal** to  $\pi$  conduction electrons  $\mapsto J=0$

➤  $p_z$  state – **Ferromagnetic** coupling  $\mapsto J=0$

$J=0 \mapsto$  NO KONDO SCREENING

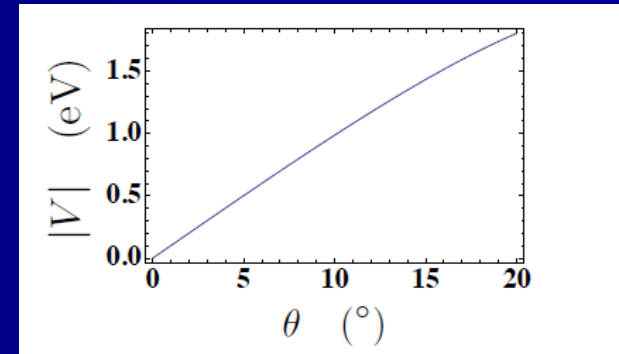
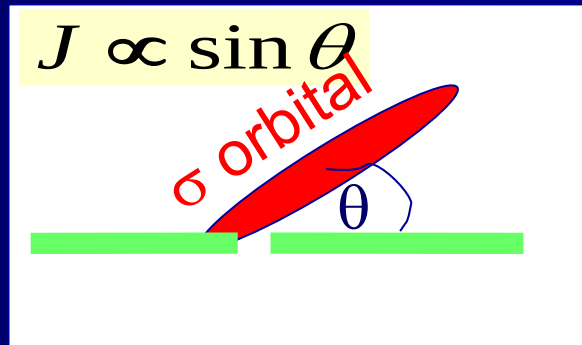
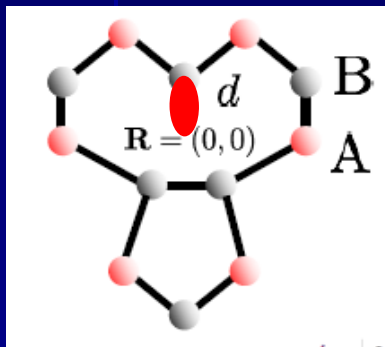


# What determines $J$

## Local Moment Formation and Kondo Effect in Defective Graphene

M. A. Cazalilla,<sup>1,2</sup> A. Iucci,<sup>3</sup> F. Guinea,<sup>4</sup> and A. H. Castro Neto<sup>2</sup>

- Out of plane distortion of dangling bond
- ↳ Finite AF coupling with conduction electrons ↳ Kondo screening



Need Corrugated Substrate

$J$  strongly depends on Local curvature

↳ not all moments screened

↳ Need local measurement to observe Kondo screening



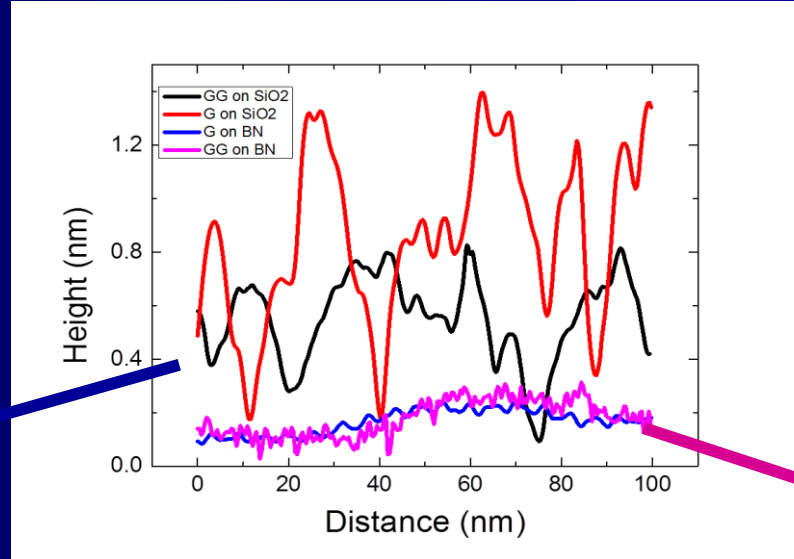
# Substrate corrugation and Kondo screening

G/SiO<sub>2</sub>

G/G/SiO<sub>2</sub>

G/hBN

G/G/hBN



G/G/SiO<sub>2</sub>

1 nm

0 nm

G/G/hBN

***J depends on Local corrugation***

⇒ not all moments screened

⇒ Global measurements can mislead

# Summary

## □ Vacancy moment and Kondo screening

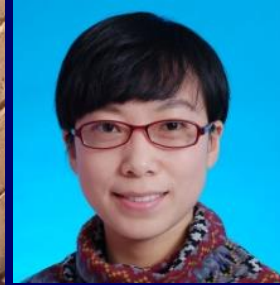
- Screening depends on local corrugation → not all moments screened
- Magnetization: only sensitive to unscreened moments
- Transport and STM: only sensitive to screened moments
- Global measurements of randomly distributed moments are misleading!
- Electrostatic control of vacancy moment



Guohong Li



Jinhai Mao



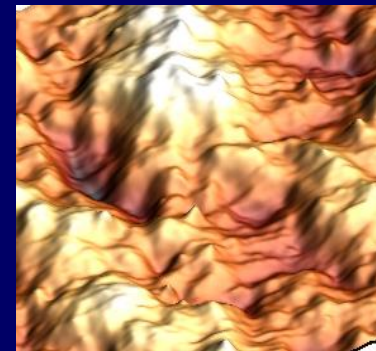
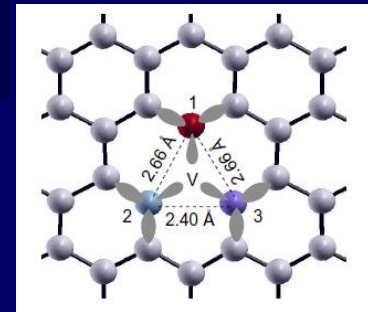
Yuhang Jiang

### Theory: (Kondo)

- D. May, F. Anders
- GY Guo, P.W Lo

### Substrates: (hBN)

- T. Taniguchi
- K. Watanabe



J. Mao et al arXiv:1711.06942

Quantum Critical Transition and Kondo Screening of Magnetic Moments in Graphene

