

# Superconductivity, pseudogap and Mott transition

A.-M. Tremblay

G. Sordi, K. Haule, P. Sémon



M2S, Washington, 2 August 2012



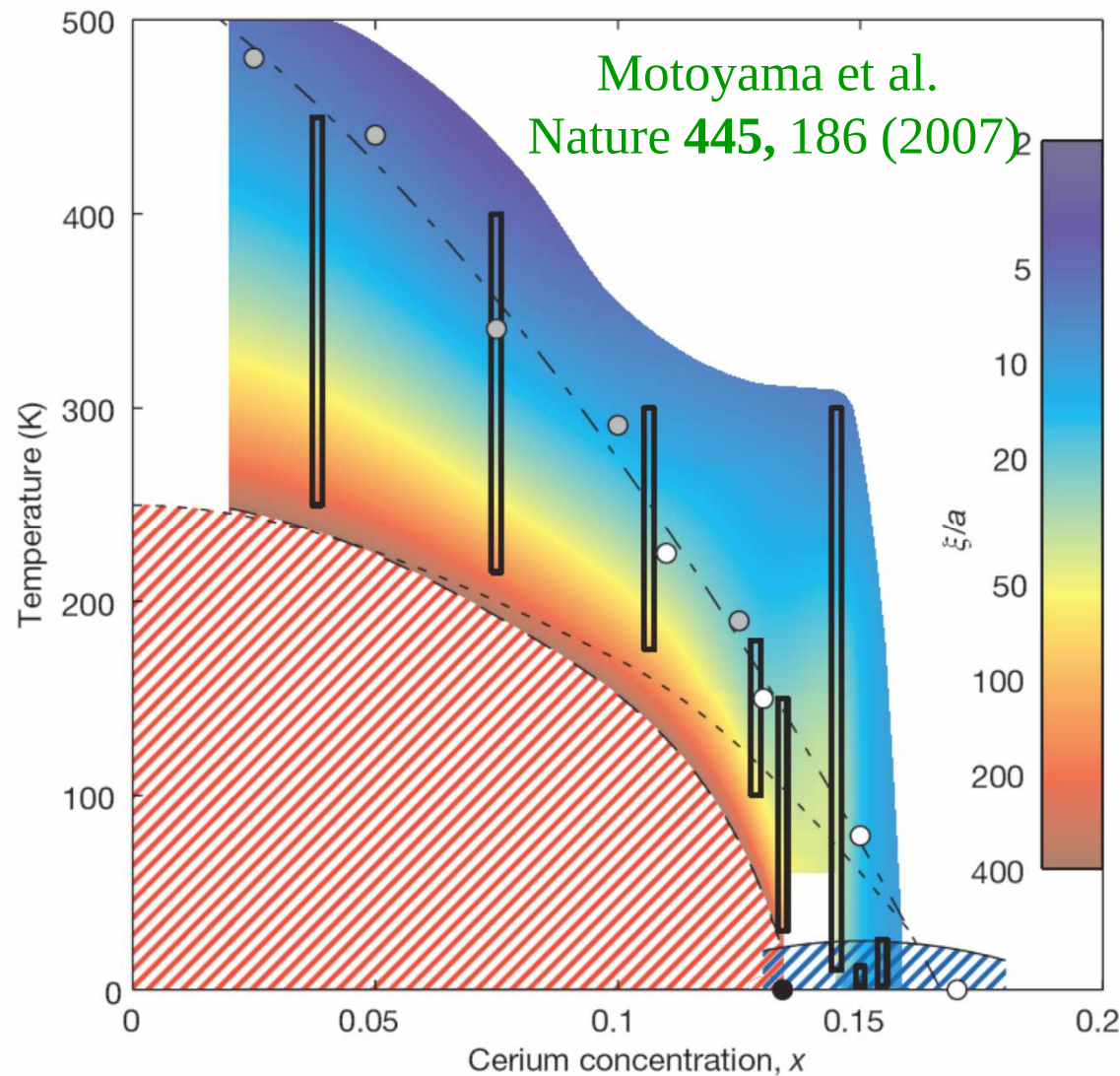
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# Three broad classes of mechanisms for pseudogap

- Rounded first order transition
- Precursor to a lower temperature broken symmetry phase
- Mott physics
- Competing order
  - Current loops: Varma, PRB **81**, 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?
  - RVB: P.A. Lee Rep. Prog. Phys. **71**, 012501 (2008)



# $d = 2$ precursors, e-doped



$$\xi^* = 2.6(2)\xi_{\text{th}}$$

Vilk, A.-M.S.T (1997)

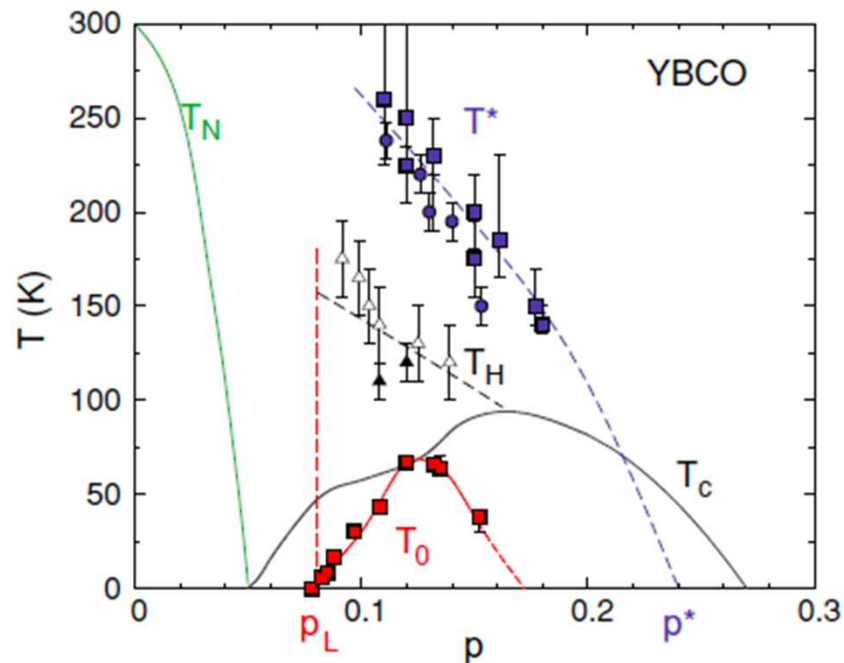
Kyung, Hankevych,  
A.-M.S.T., PRL, sept.  
2004

Semi-quantitative fits of  
both ARPES and  
neutron



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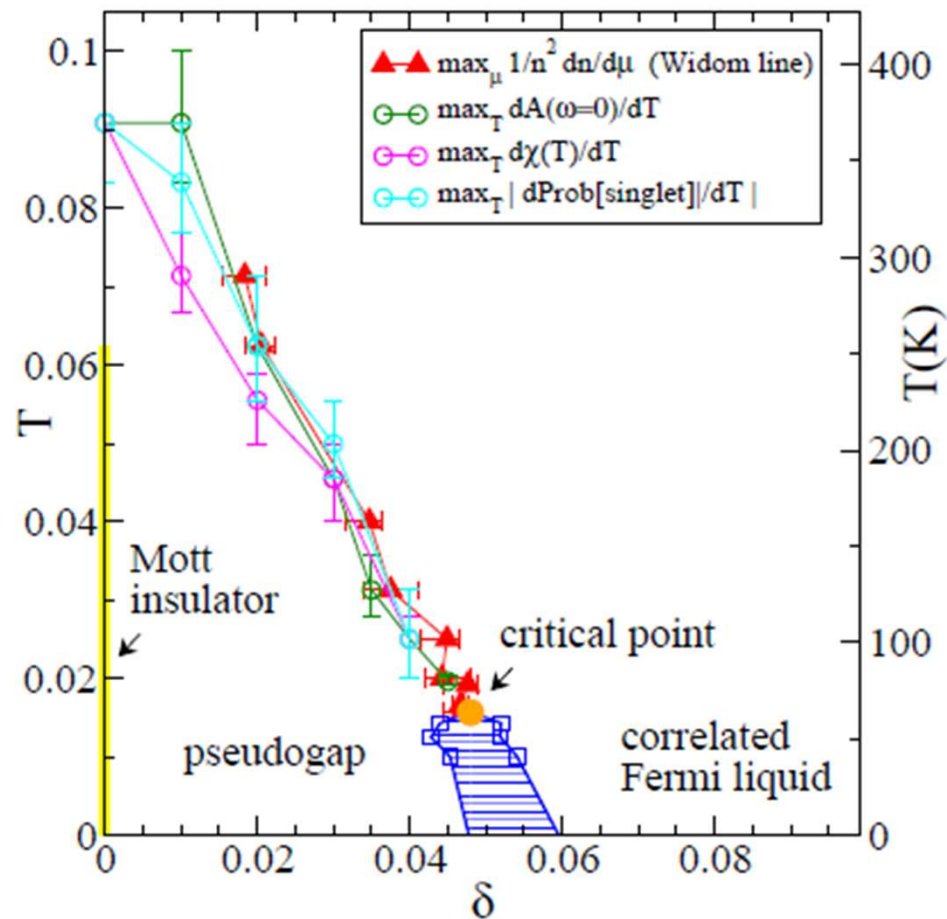
# Hole-doped case: Competing phases?



Leboeuf, Doiron-Leyraud et al. PRB **83**, 054506 (2011)



# Pseudogap from Mott physics



G. Sordi, *et al.* Scientific Reports 2, 547 (2012)

Competing order is a consequence of the pseudogap, not its cause:

Parker et al. Nature 468, 677 (2010)



# Model

$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



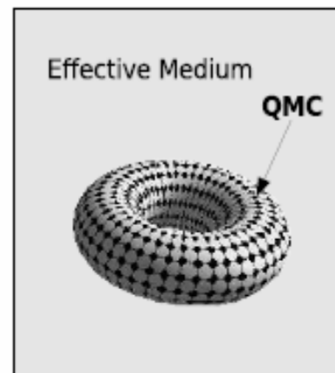
# Outline

- Method
- Finite  $T$  phase diagram
  - Normal state (no LRO, what is below the dome)
    - First order transition
    - Widom line and pseudogap
  - Superconductivity

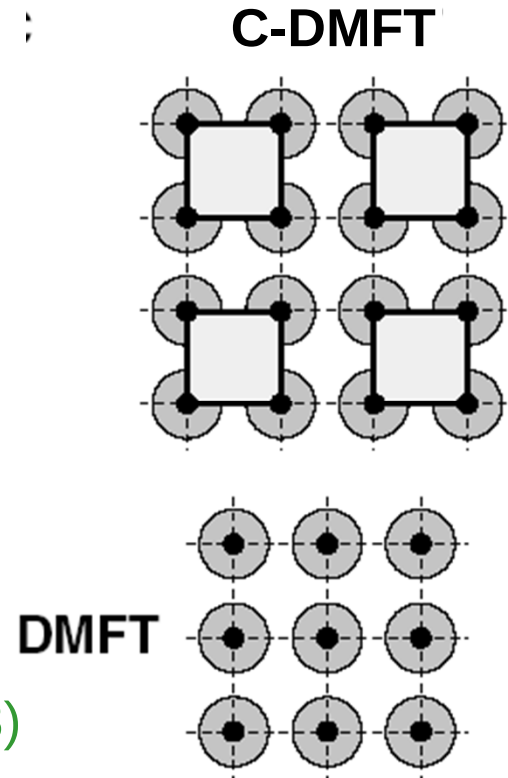


# Method

# 2d Hubbard: Quantum cluster method



DCA



Hettler ...Jarrell...Krishnamurty PRB **58** (1998)

Kotliar et al. PRL **87** (2001)

M. Potthoff *et al.* PRL **91**, 206402 (2003).

## REVIEWS

Maier, Jarrell et al., RMP. (2005)

Kotliar *et al.* RMP (2006)

AMST *et al.* LTP (2006)



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## + and -

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations



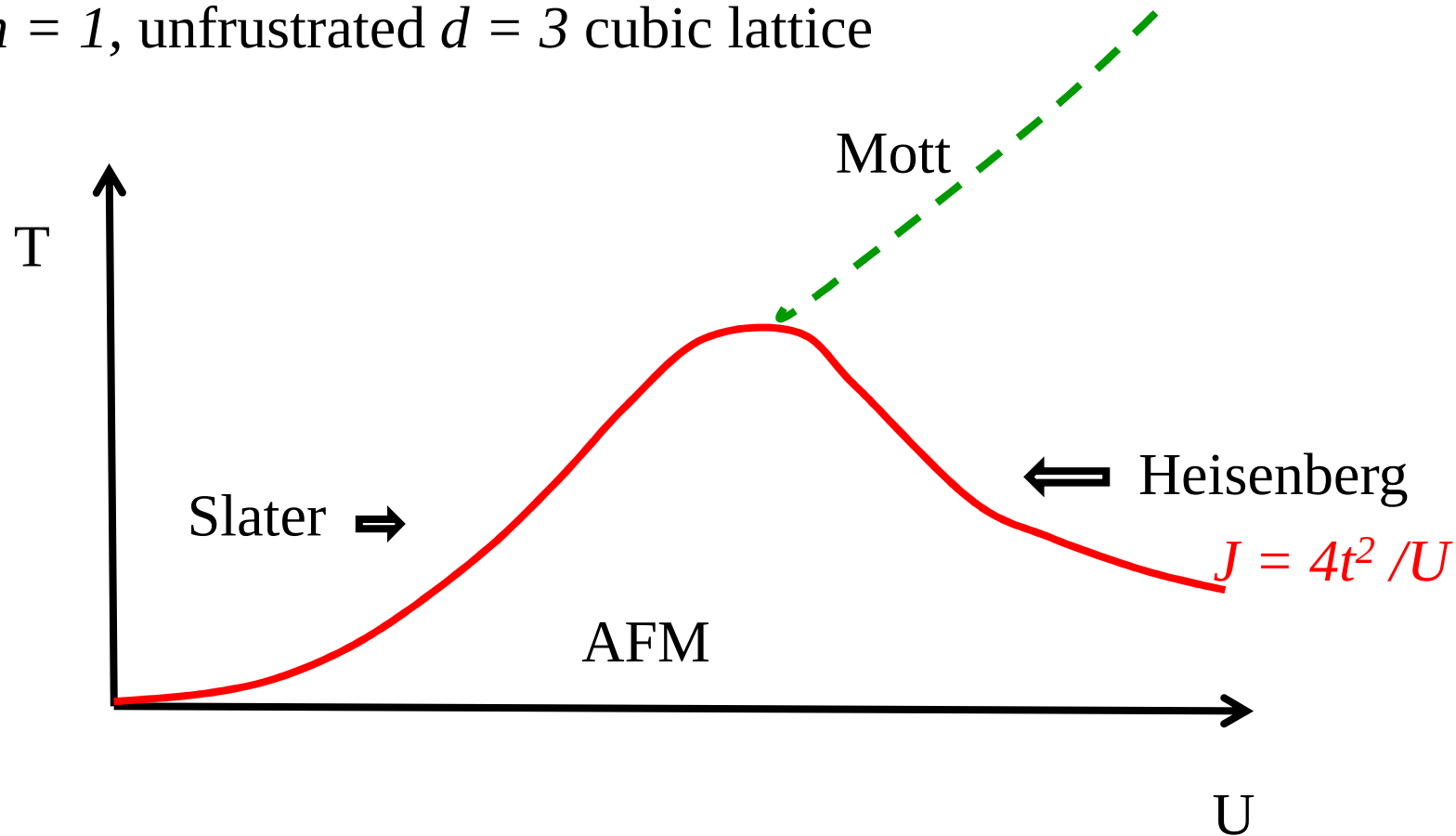
# When is cluster DMFT OK?

## Example: The Mott transition



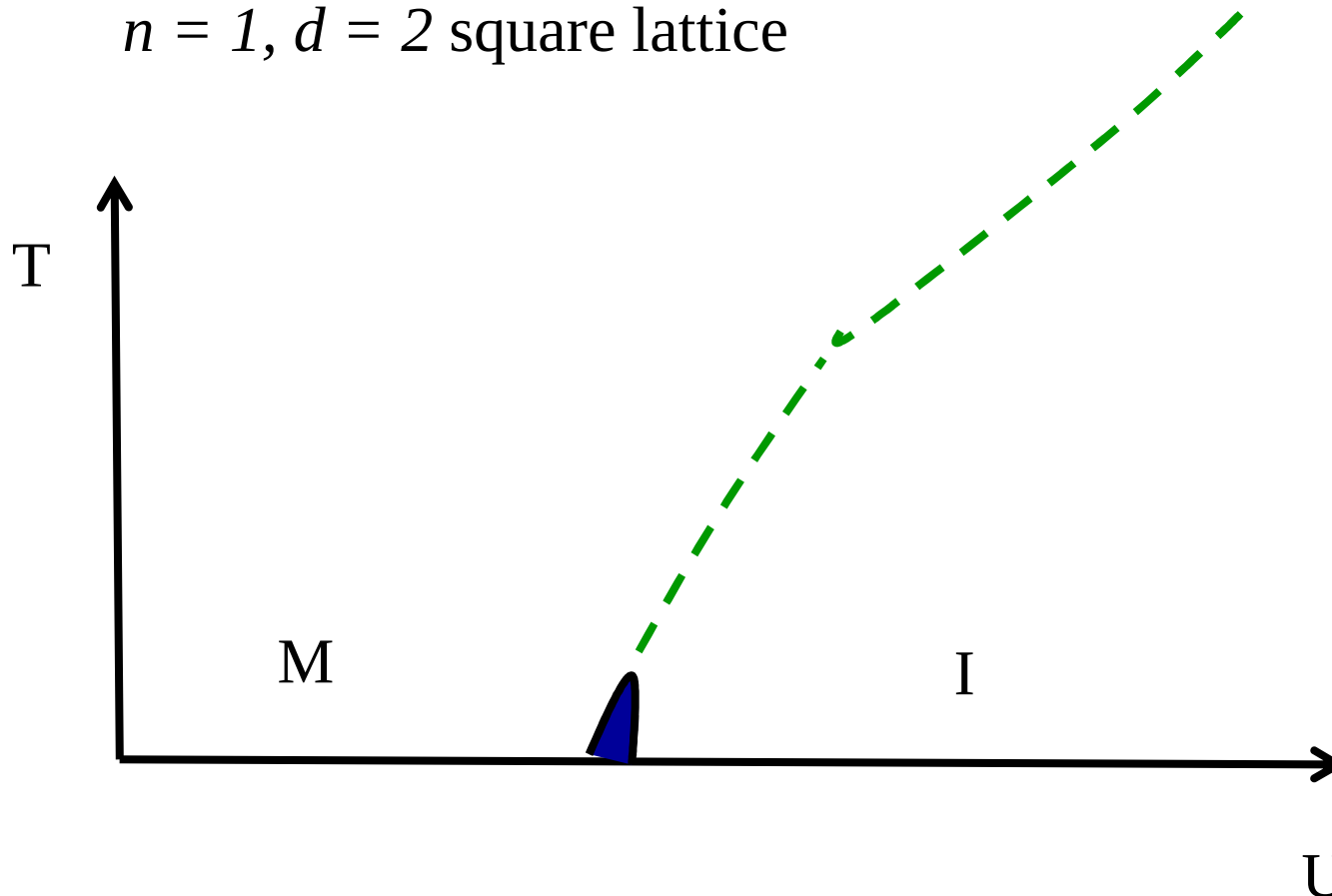
# Local moment and Mott transition

$n = 1$ , unfrustrated  $d = 3$  cubic lattice



# Local moment and Mott transition

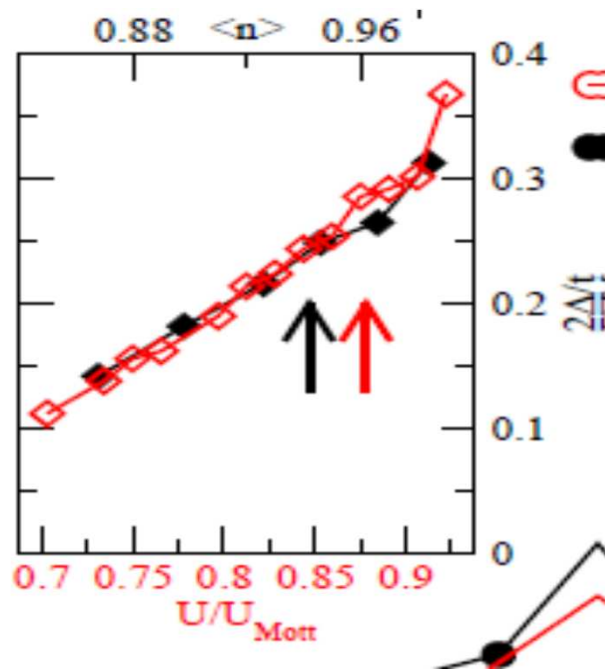
$n = 1, d = 2$  square lattice



Understanding finite temperature phase from a *mean-field theory* down to  $T = 0$



# Size dependence



Gull, Parcollet, Millis  
arXiv:1207.2490v1

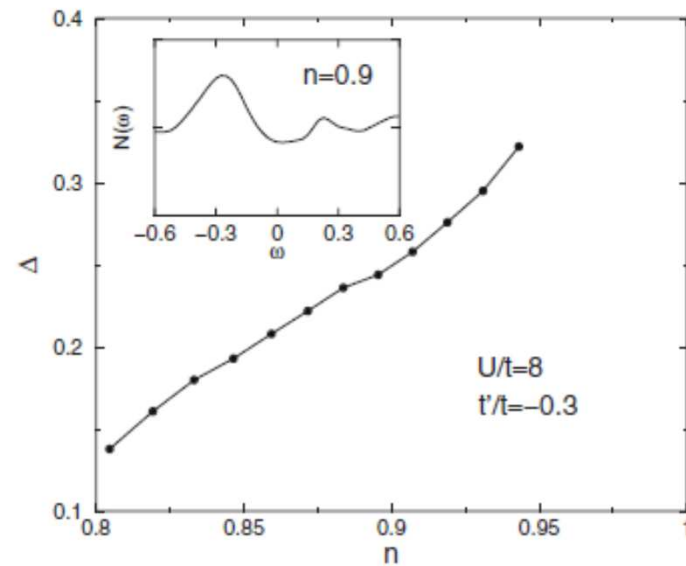
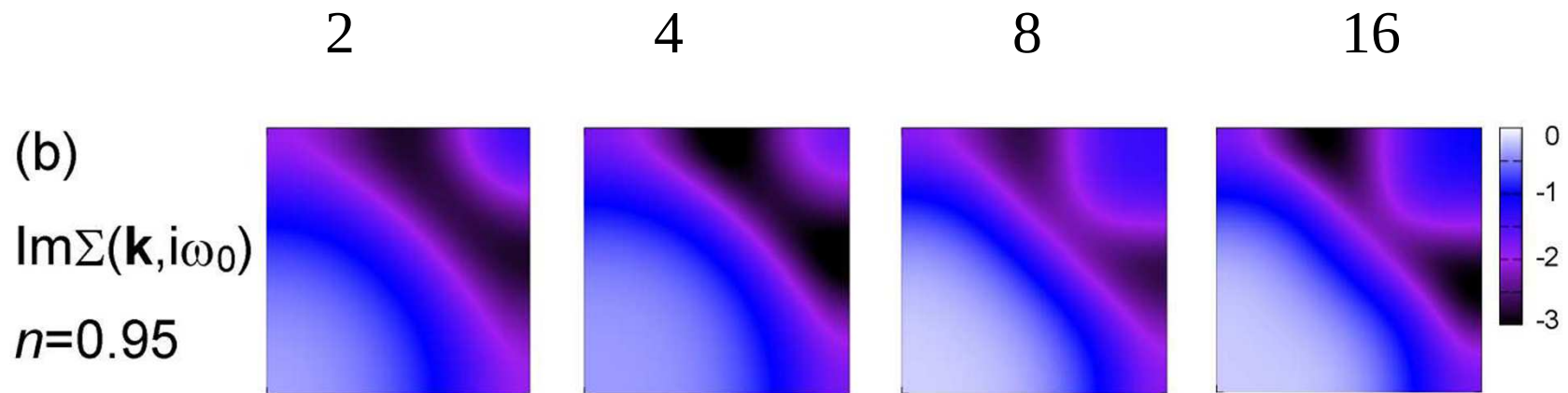


FIG. 5. The gap as a function of filling, for  $U=8t$ ,  $t'=-0.3t$ . The gap is defined as half the distance between the two peaks on either side of  $\omega=0$ , as they appear, for example, in the inset.

Kancharla et al. PRB 77, 184516 (2008)

# Size dependence near FS



Sakai et al. arXiv:1112.3227



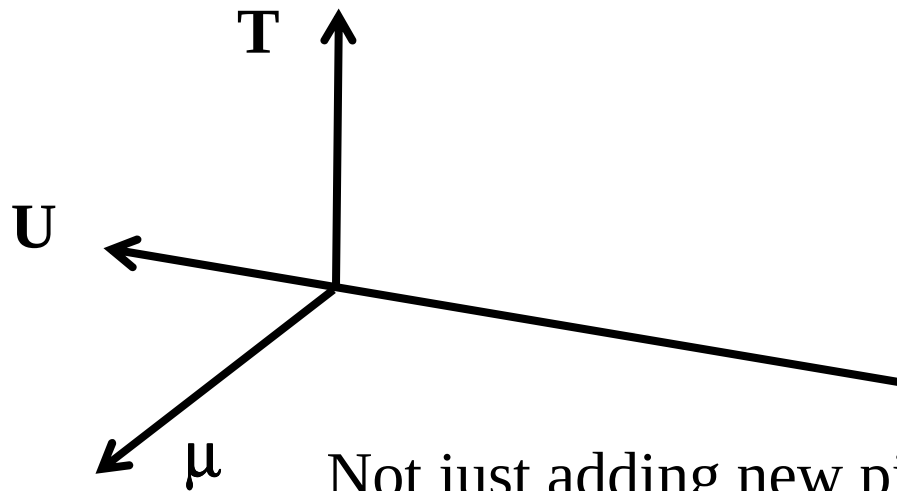
Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T  
PRL, **104**, 226402 (2010)

and

Phys. Rev. B. **84**, 075161 (2011)

## Doping-induced Mott transition ( $t'=0$ )



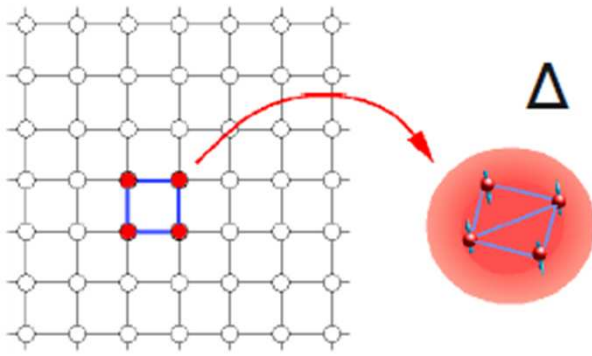
Kristjan Haule

Not just adding new piece:  
Lesson from DMFT, first order transition + critical  
point governs phase diagram



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# C-DMFT



Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006

P. Werner, PRB 2007

K. Haule, PRB 2007

$$Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger(\tau) \Delta_{\mathbf{k}}(\tau, \tau') \psi_{\mathbf{k}}(\tau')}$$

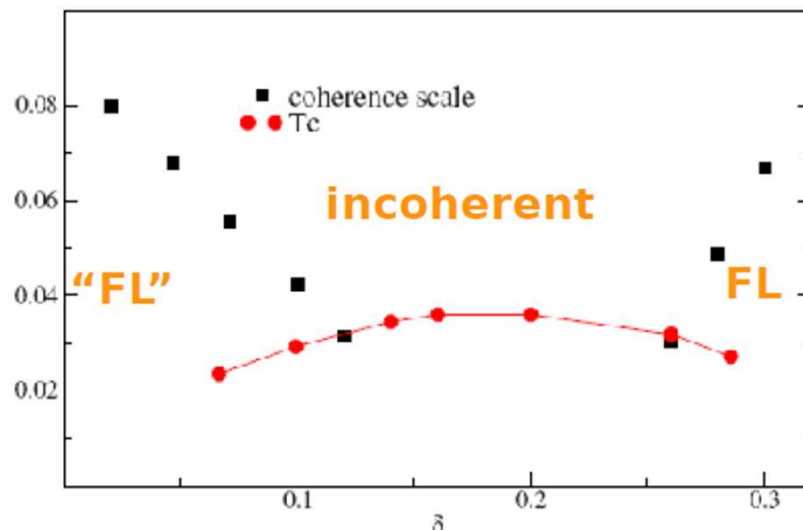
Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

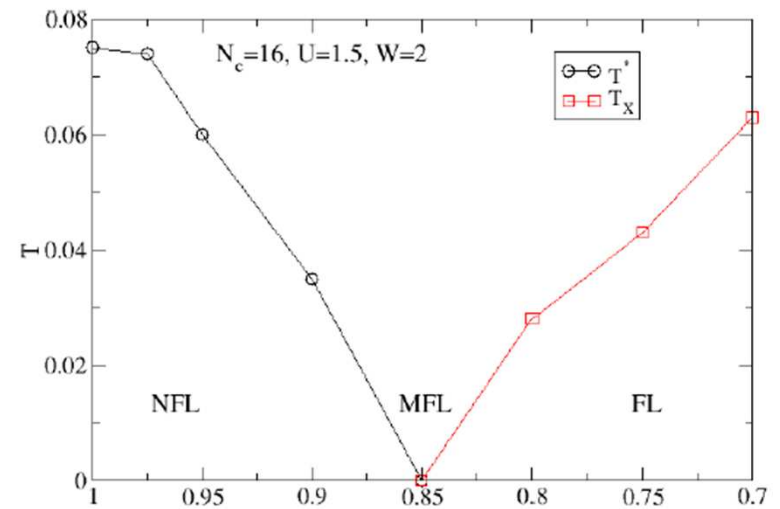
K. Haule, Phys. Rev. B **75**, 155113 (2007).

# Doping driven Mott transition, $t' = 0$

| Method  | $t'$ | Orbital selective | U    | Critical point | Ref.                          |
|---------|------|-------------------|------|----------------|-------------------------------|
| D+C+H 8 |      |                   | 7    |                | Werner et al. cond-mat (2009) |
| D+C+H 4 |      |                   |      |                | Gull et al. EPL (2008)        |
|         | -0.3 |                   | 10,6 |                | Liebsch, Merino... (2008)     |
|         |      |                   |      |                | Ferrero et al. PRB (2009)     |
| D+C+H 8 |      |                   | 7    |                | Gull, et al. PRB (2009)       |

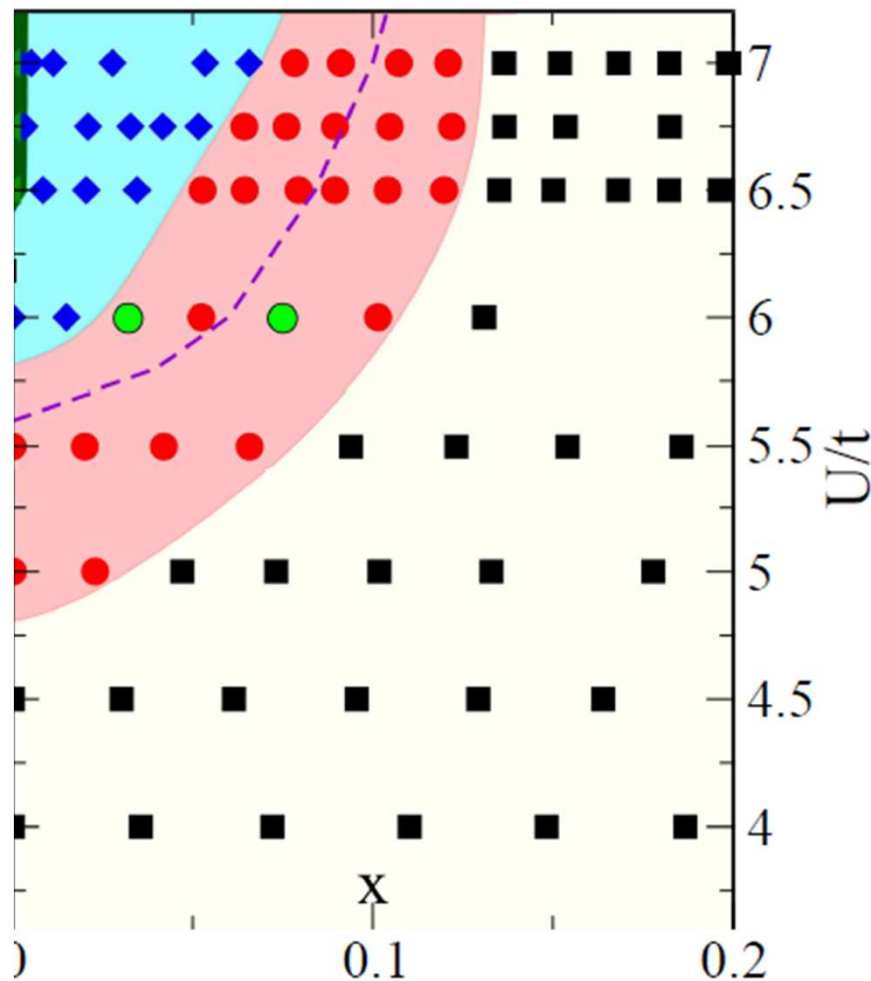


K. Haule, G. Kotliar, PRB (2008)



Vildhyadhiraja, PRL (2009)

# Doping driven Mott transition



$$T = 0.25 t$$

Gull, Parcollet, Millis  
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)

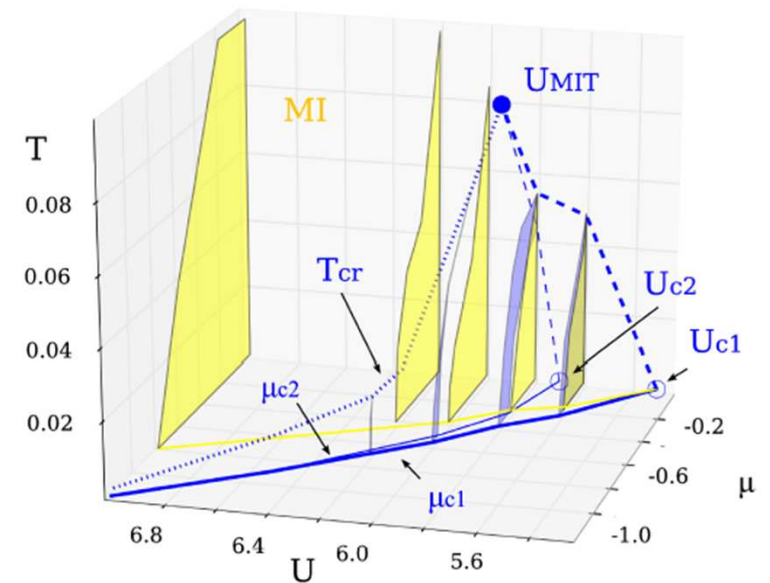
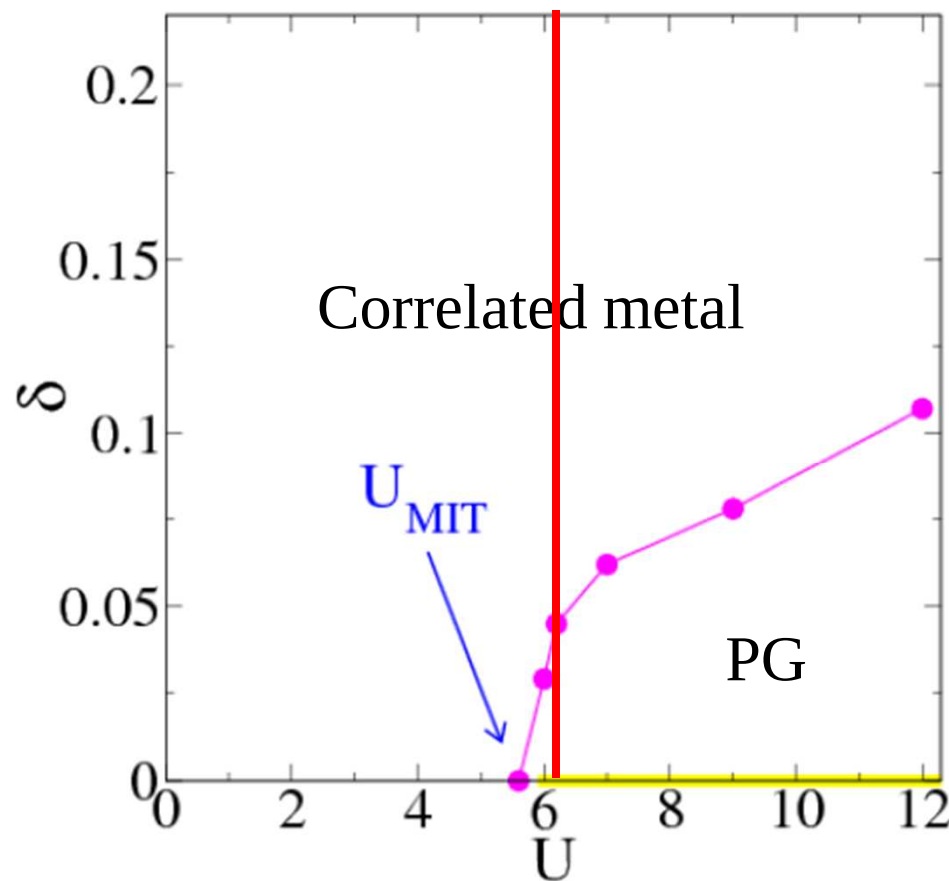
E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis (2010)



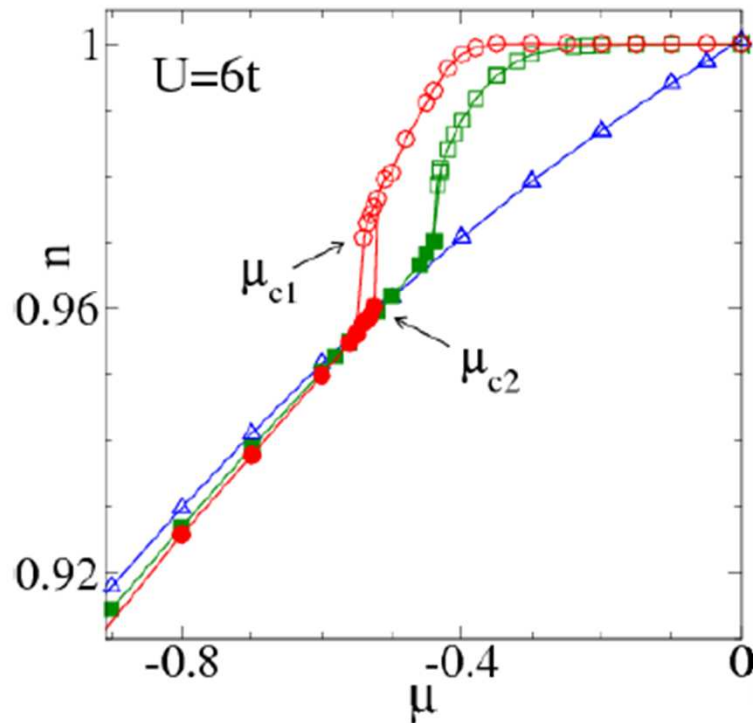
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# Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of  $U$



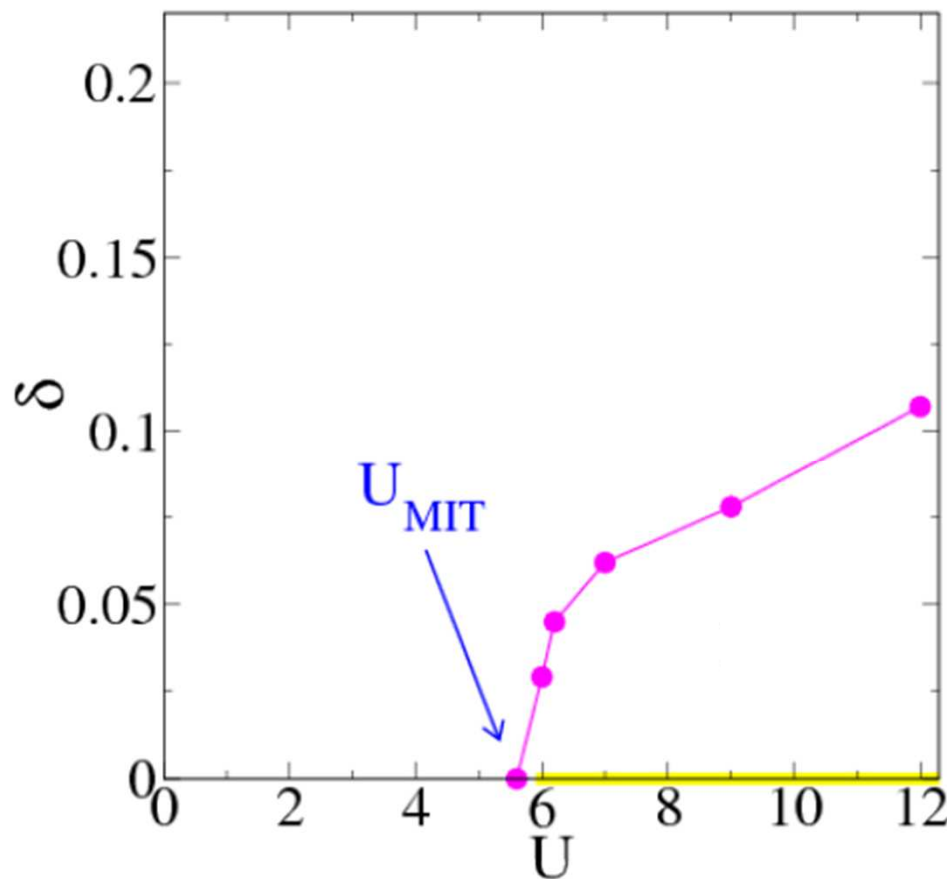
# First order transition at finite doping



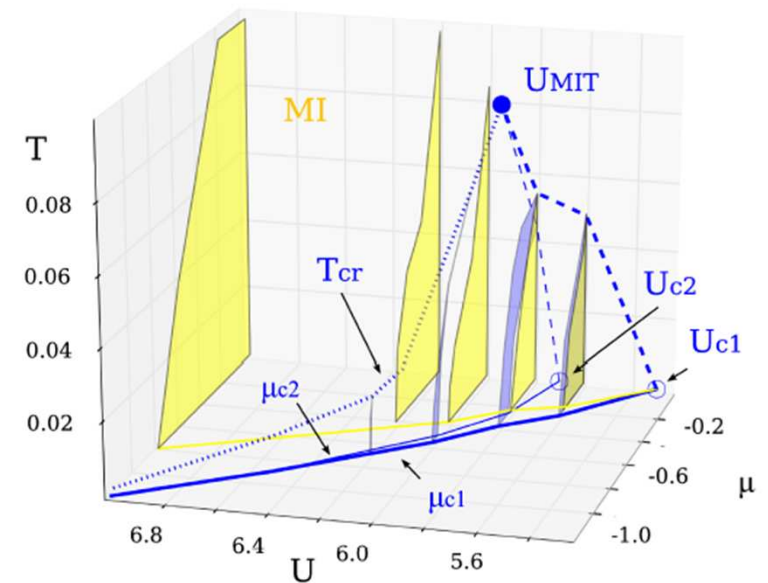
$n(\mu)$  for several temperatures:  
 $T/t = 1/10$ ,  $1/25$ ,  $1/50$

# Link to Mott transition up to optimal doping

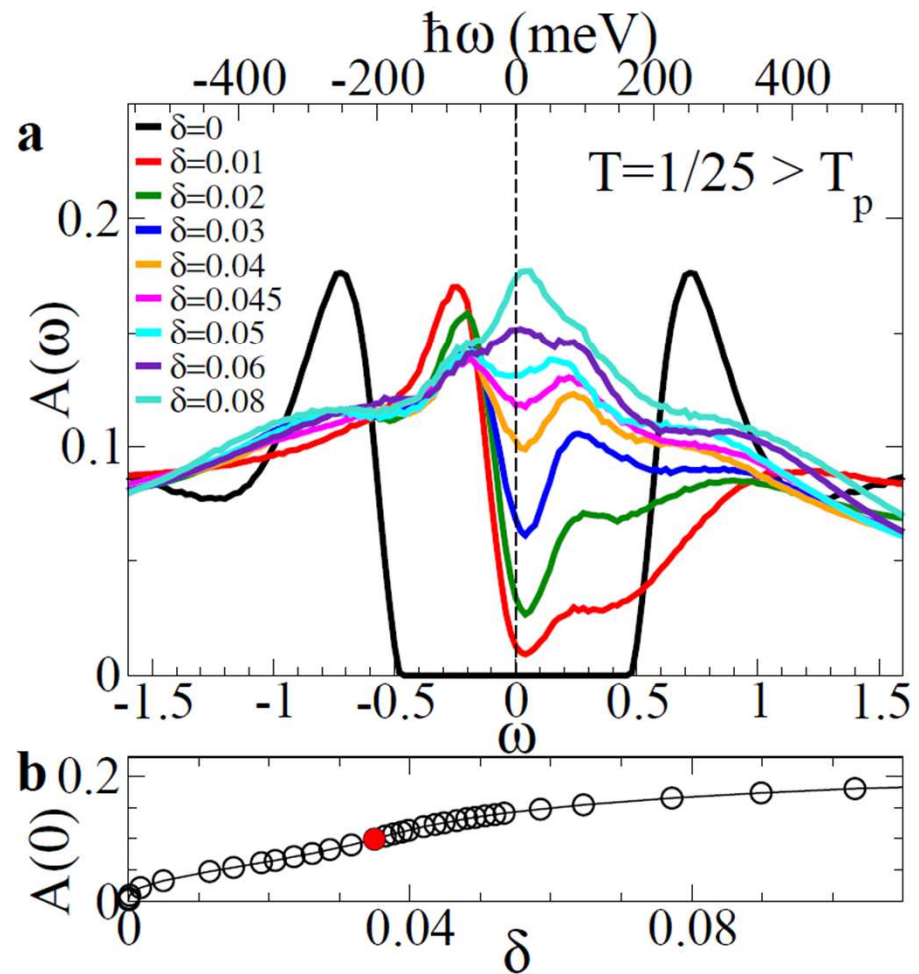
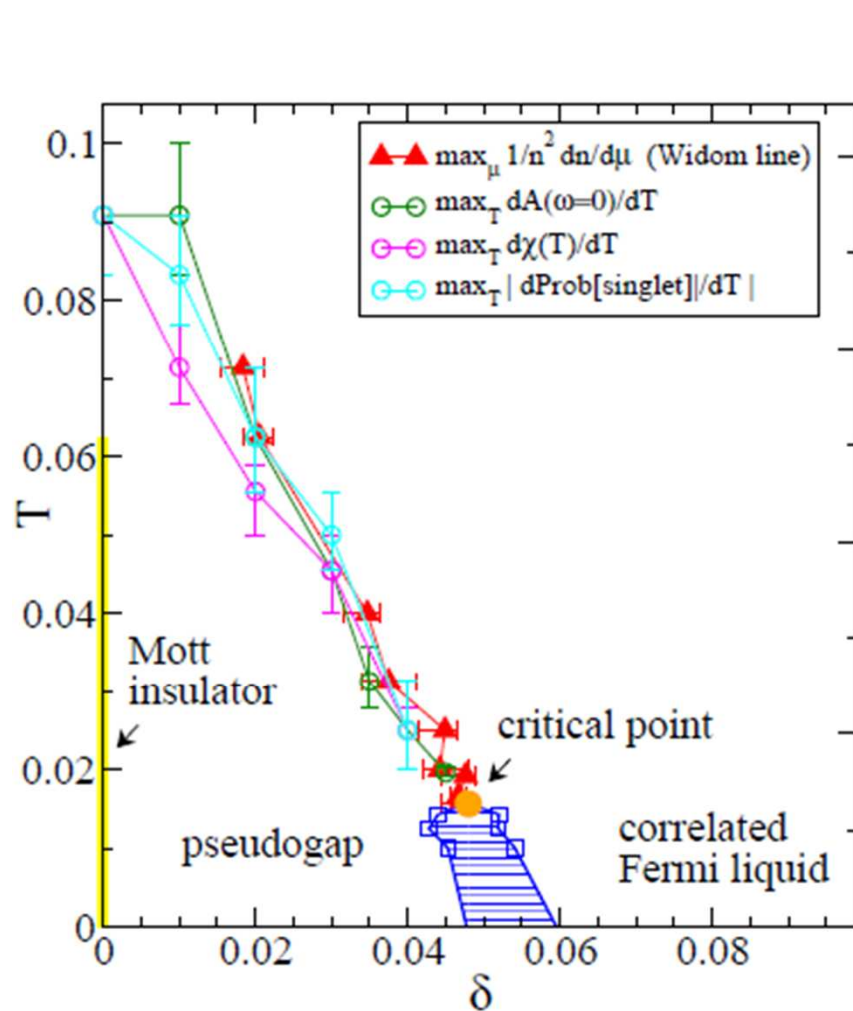
Doping dependence of critical point as a function of  $U$



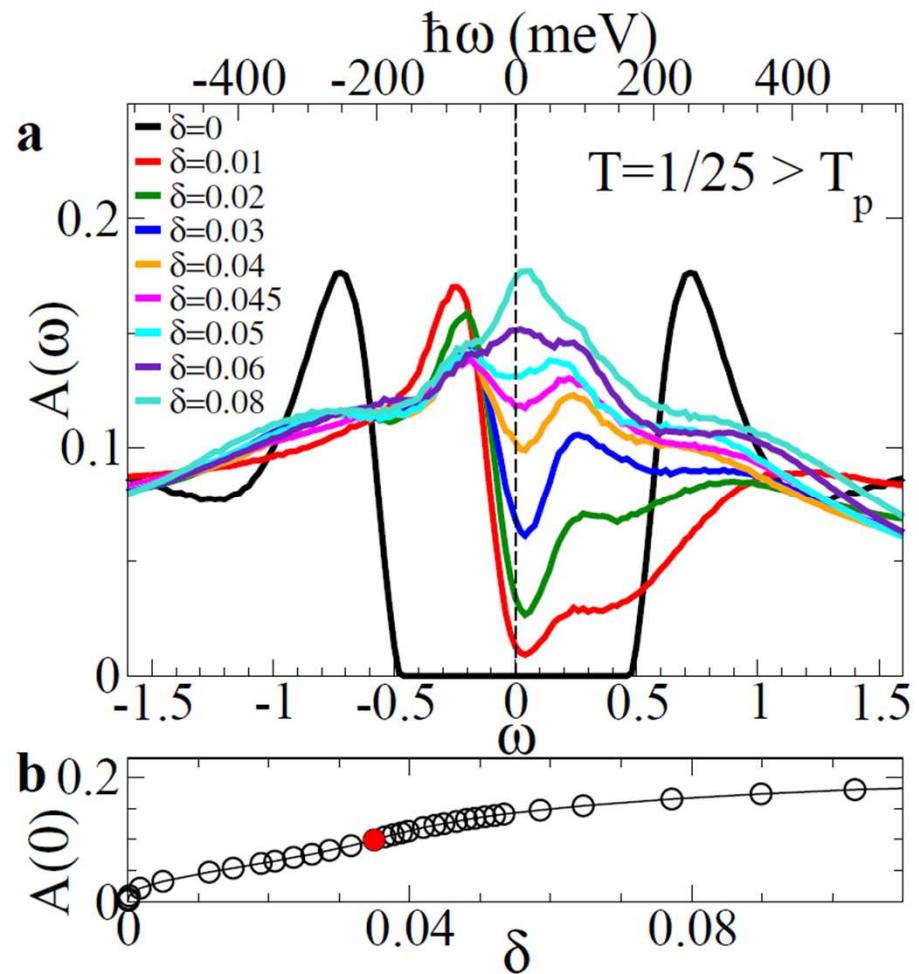
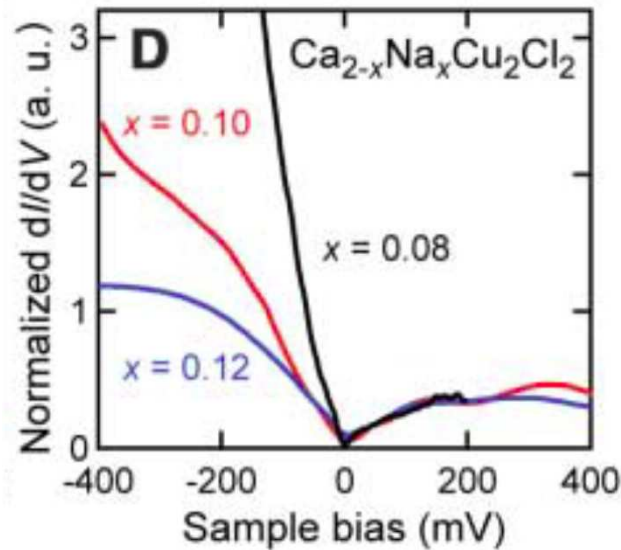
Smaller  $D$  and  $S$



# Density of states

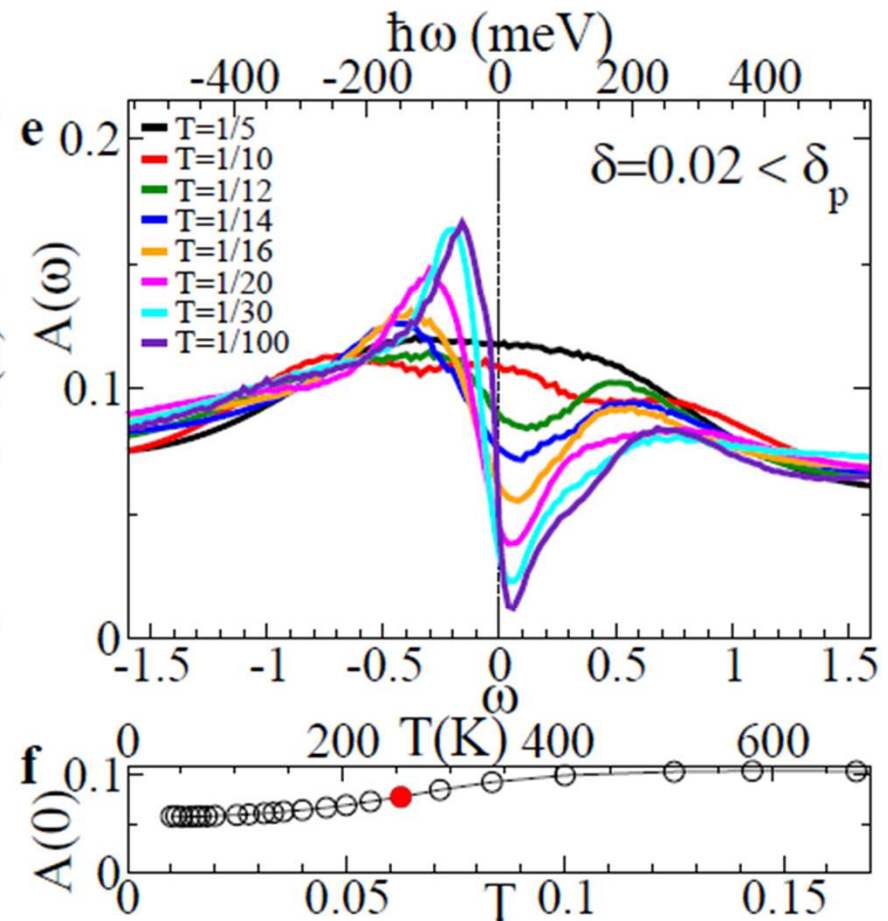
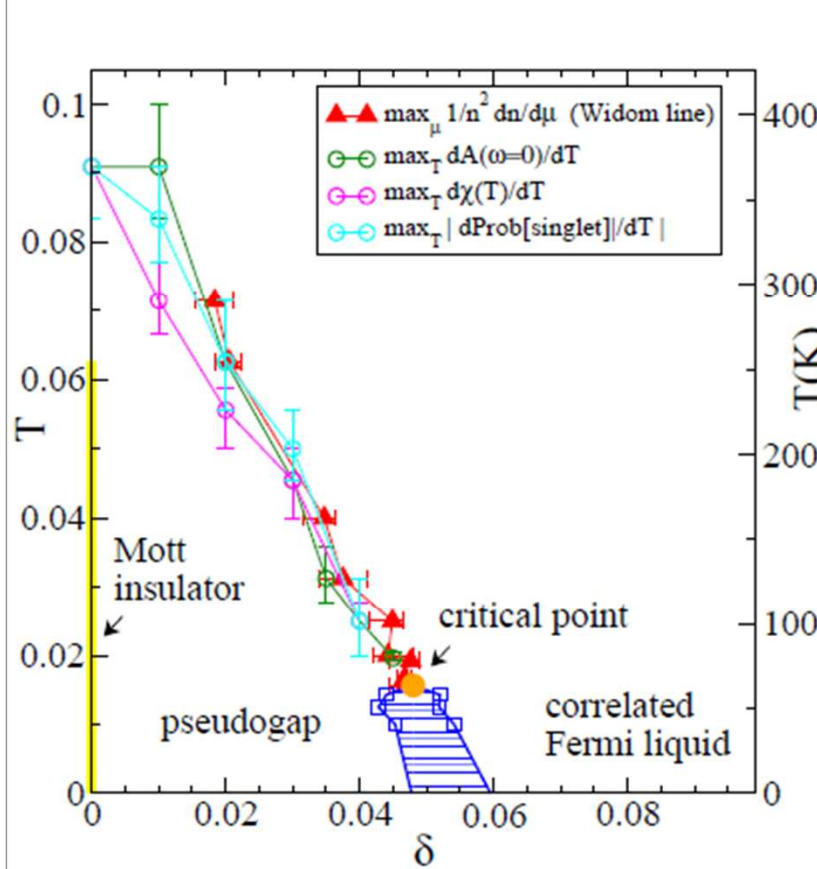


# Density of states

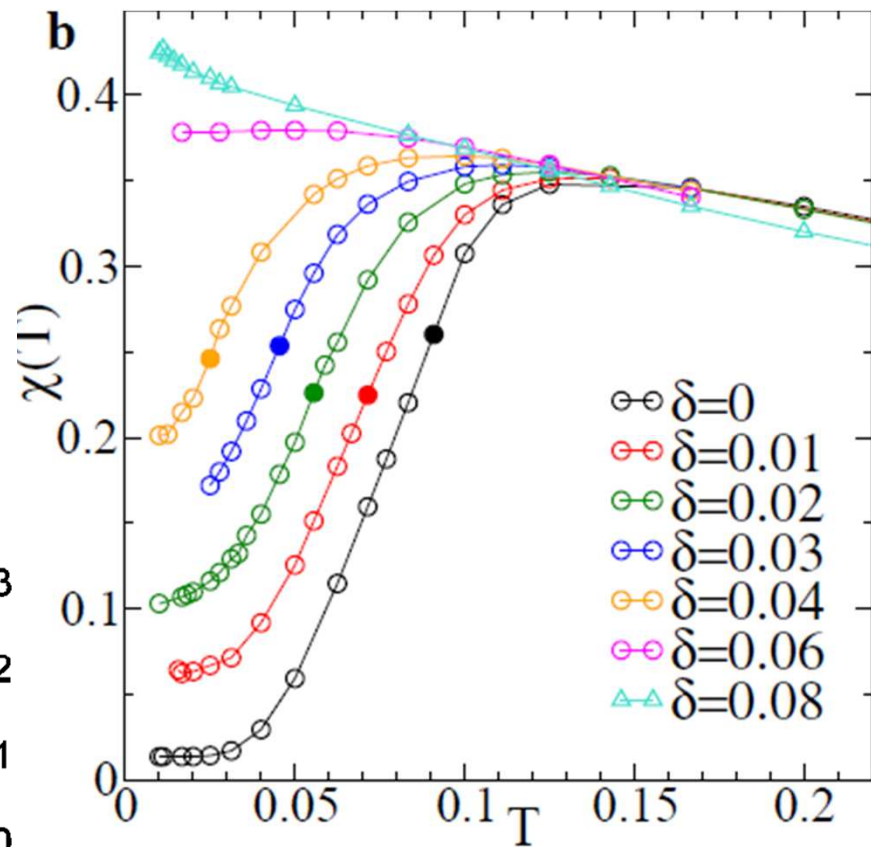
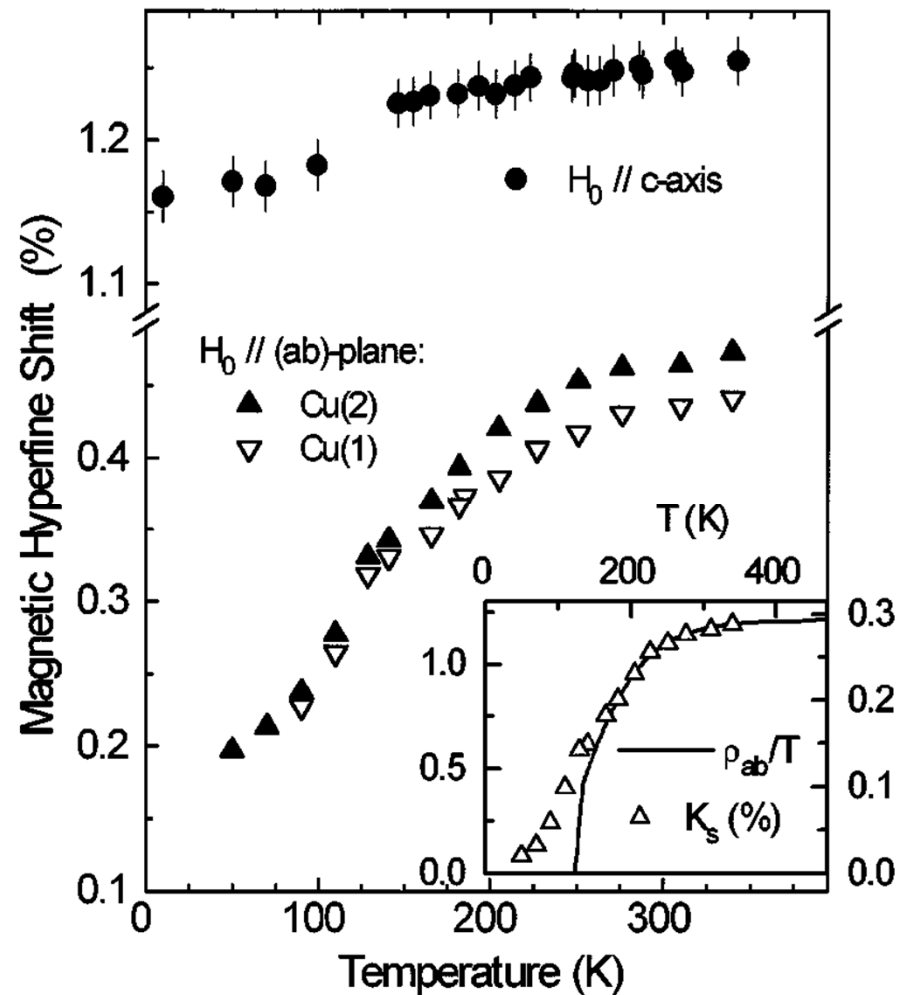


Khosaka et al. *Science* **315**, 1380 (2007);

# Density of states



# Spin susceptibility



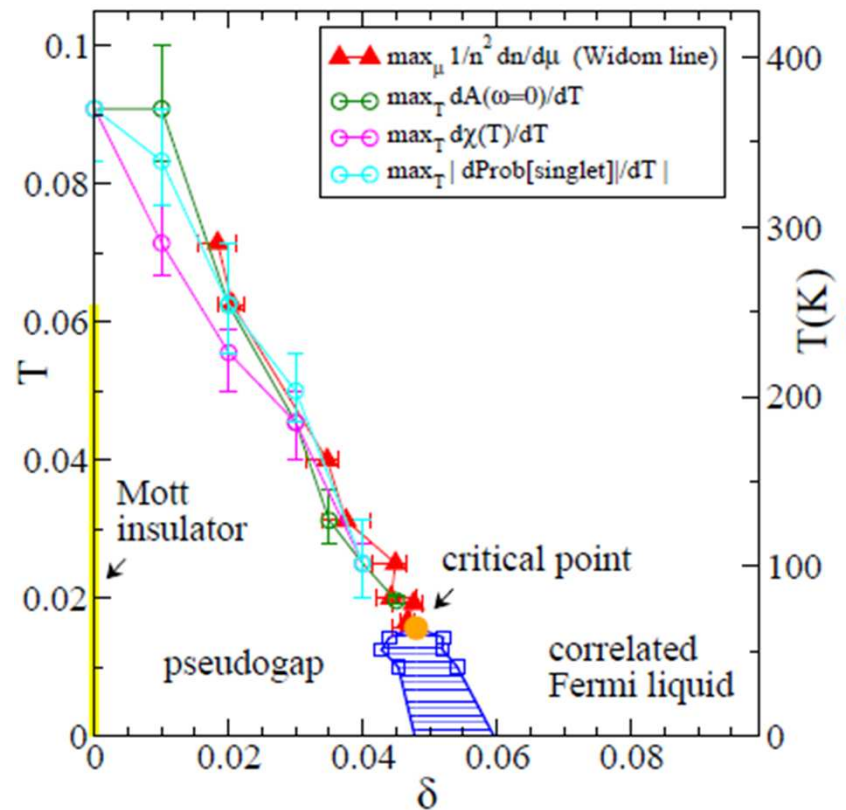
Underdoped Hg1223

Julien et al. PRL **76**, 4238 (1996)



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# Pseudogap $T^*$ along the Widom line





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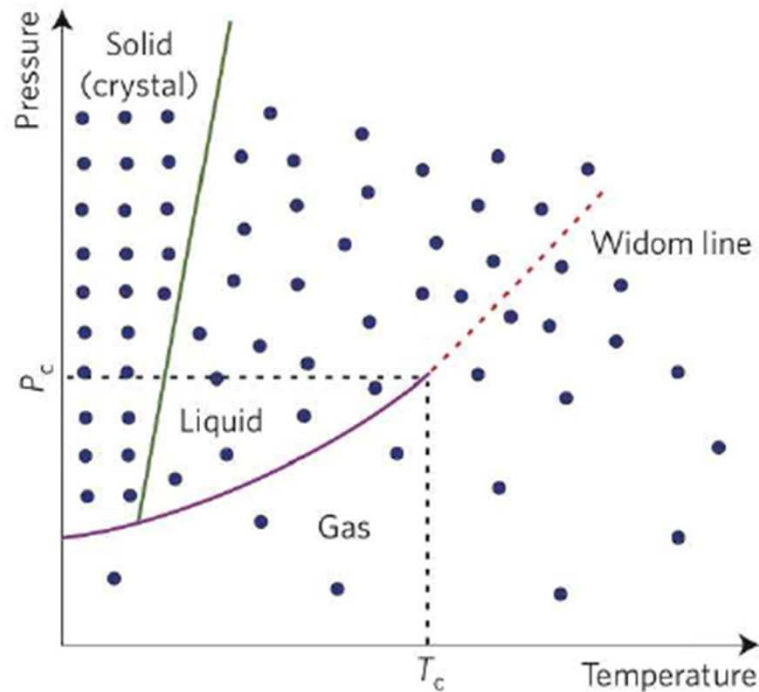
# The Wisdom line

G. Sordi, *et al.* Scientific Reports 2, 547 (2012)



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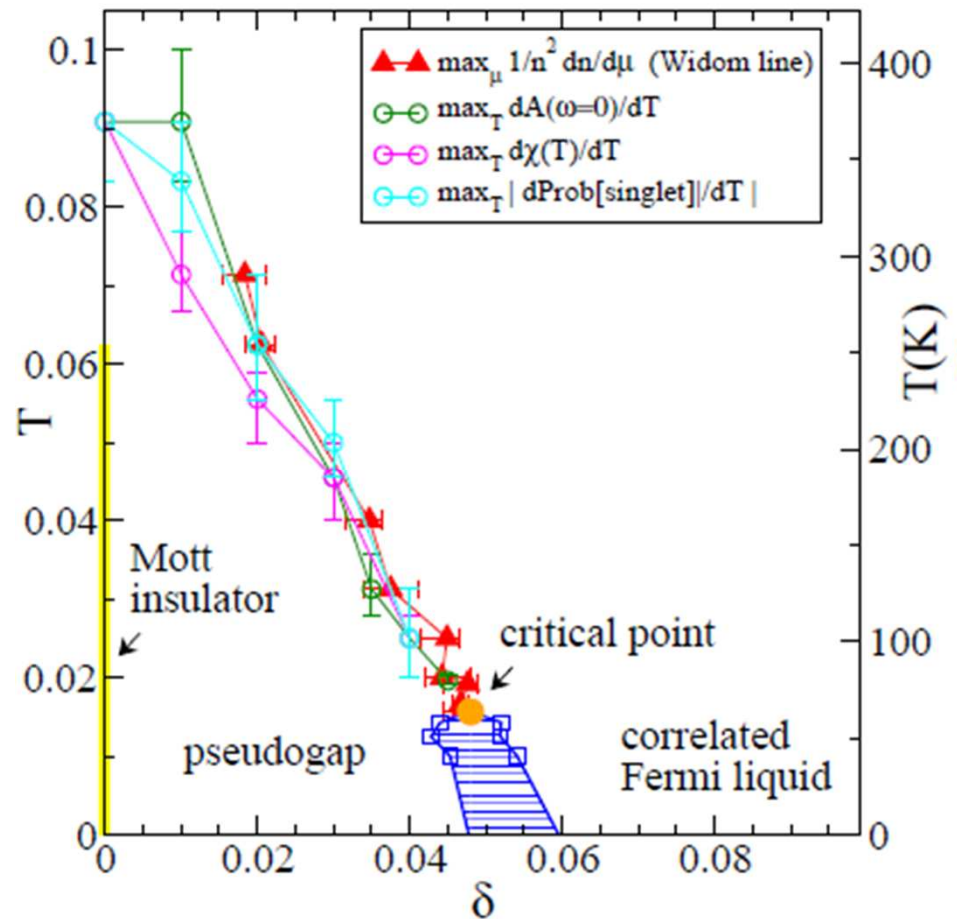
# What is the Widom line?



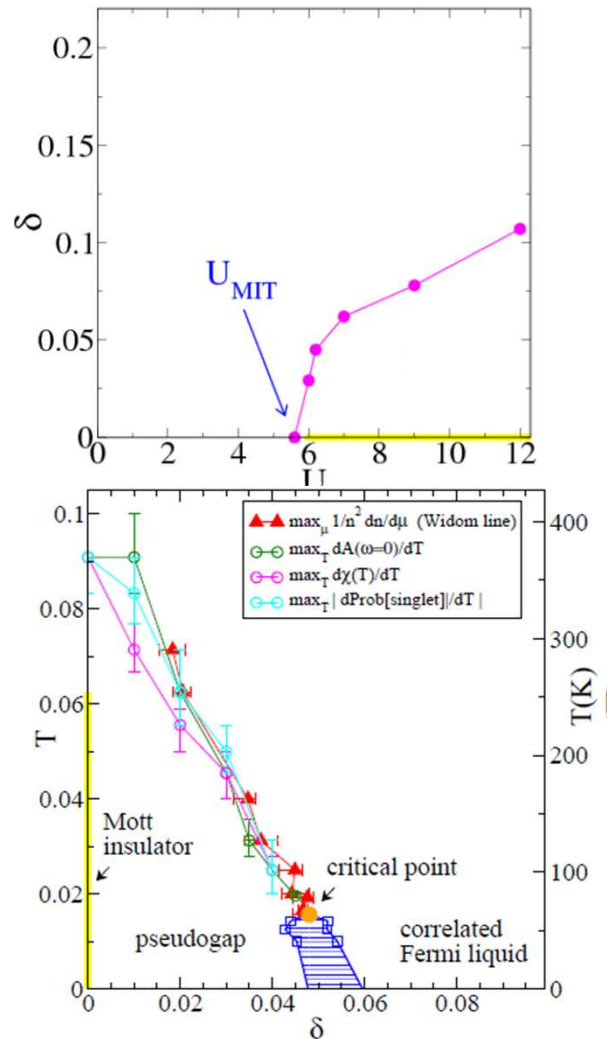
McMillan and Stanley, Nat Phys 2010

- ▶ it is the continuation of the coexistence line in the supercritical region
- ▶ line where the **maxima of different response functions** touch each other asymptotically as  $T \rightarrow T_p$
- ▶ liquid-gas transition in water: max in isobaric heat capacity  $C_p$ , isothermal compressibility, isobaric heat expansion, etc
- ▶ **DYNAMIC crossover arises from crossing the Widom line!**  
water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

# Phase diagram



# Summary: normal state



- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap  $T^*$  is a Widom line
- High compressibility (stripes?)



Giovanni Sordi



Patrick Sémon



Kristjan Haule

# Finite $T$ phase diagram

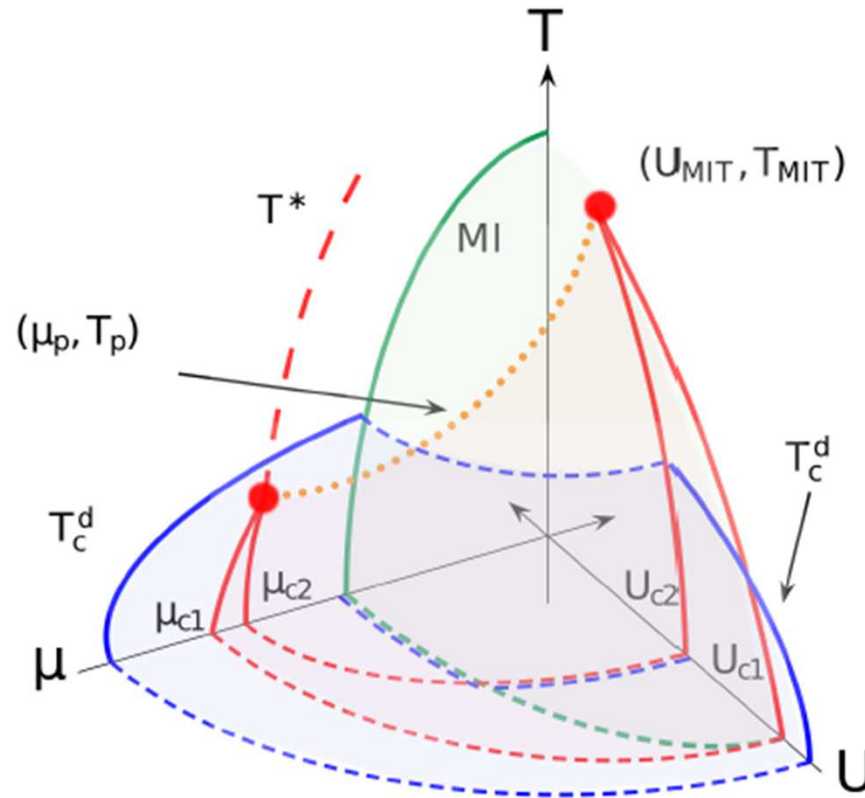
## Superconductivity

Sordi et al. PRL **108**, 216401 (2012)

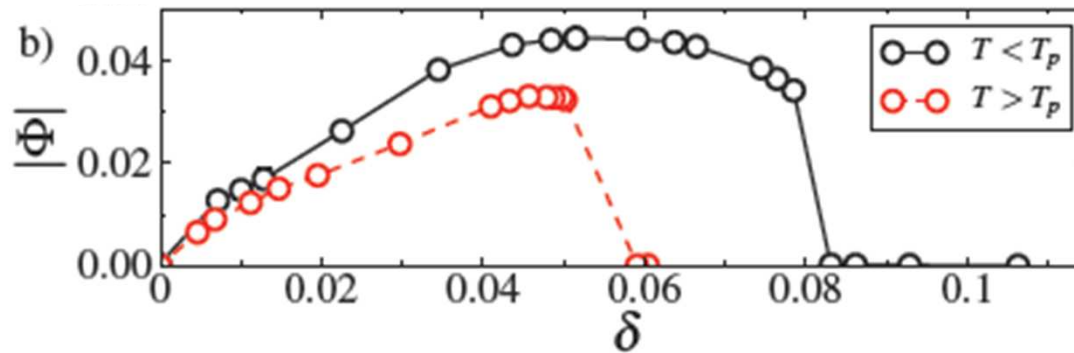


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# Unified phase diagram

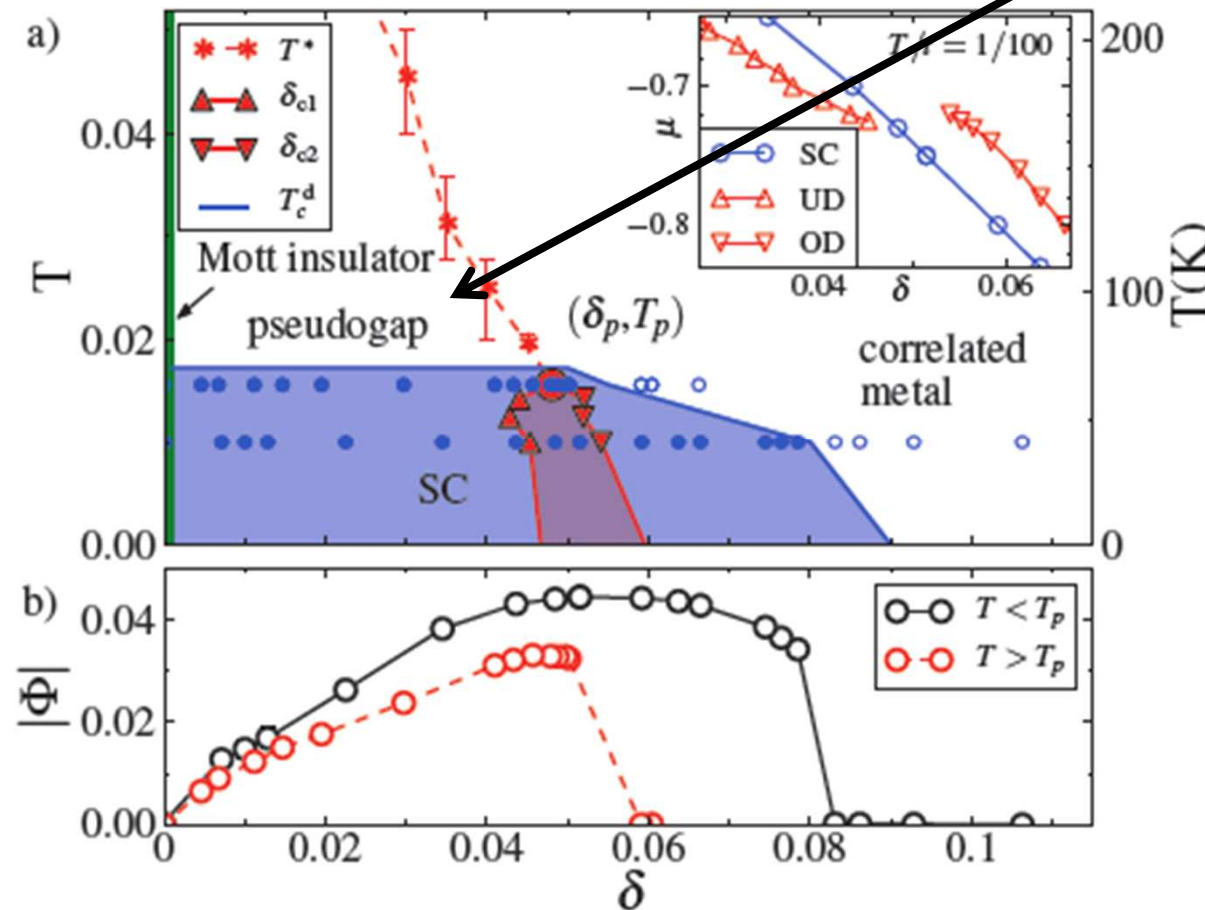


# Cuprates (doping driven transition)



# Cuprates (doping driven transition)

Pseudogap vs pair



F. Rullier-Albenque, H. Alloul, and G. Rikken, Phys. Rev. B **84**, 014522 (2011).



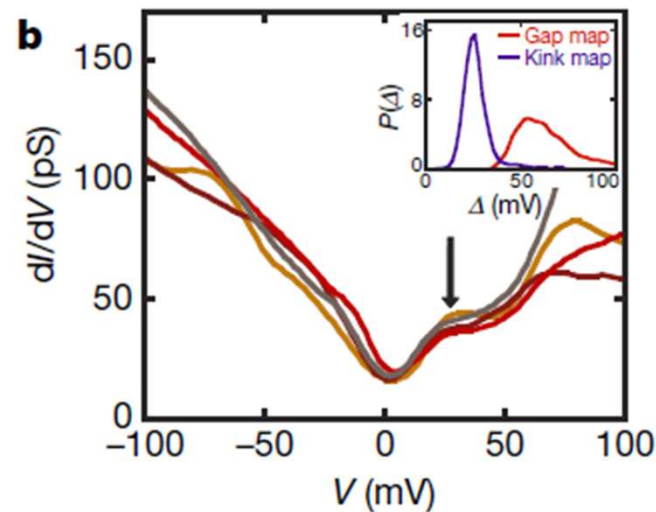
# Larger clusters

- Is there a minimal size cluster where  $T_c$  vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped



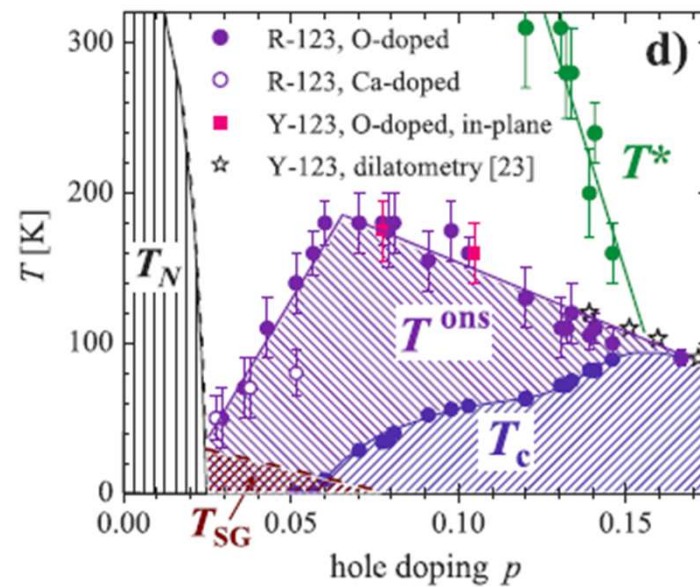
# Meaning of $T_c^d$

- Local pair formation



K. K. Gomes, A. N. Pasupathy, A. Pushp,  
S. Ono, Y. Ando, and A. Yazdani,  
Nature **447**, 569 (2007)

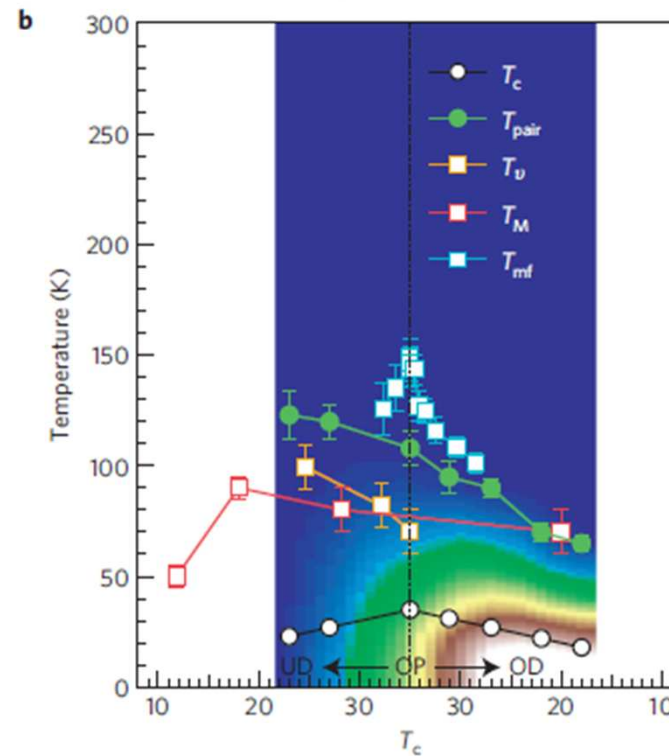
# Fluctuating region



Infrared response

Dubroka et al. 106, 047006 (2011)

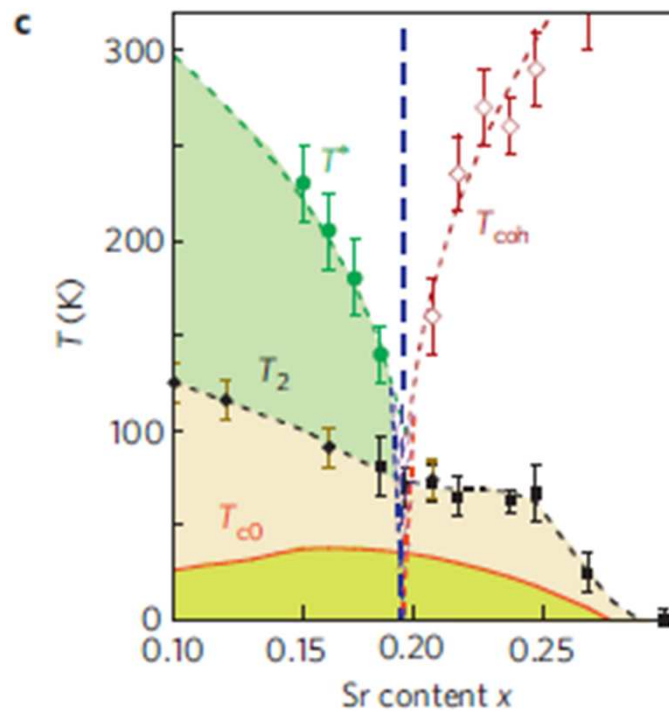
# $T_{\text{pair}}$



ARPES  
Bi2212

Kondo, Takeshi, et al. Kaminski Nature  
Physics **2011**, 7, 21-25

$$T_2$$



Magnetoresistance, LSCO  
Fluctuating vortices

Patrick M. Rourke, et al. *Nature Physics* 7, 455–458 (2011)



# Giant proximity effect

$$T_c = 32 \text{ K}$$
$$T_c < 5 \text{ K}$$

Morenzoni et al.,  
Nature Comms. 2 (2011)

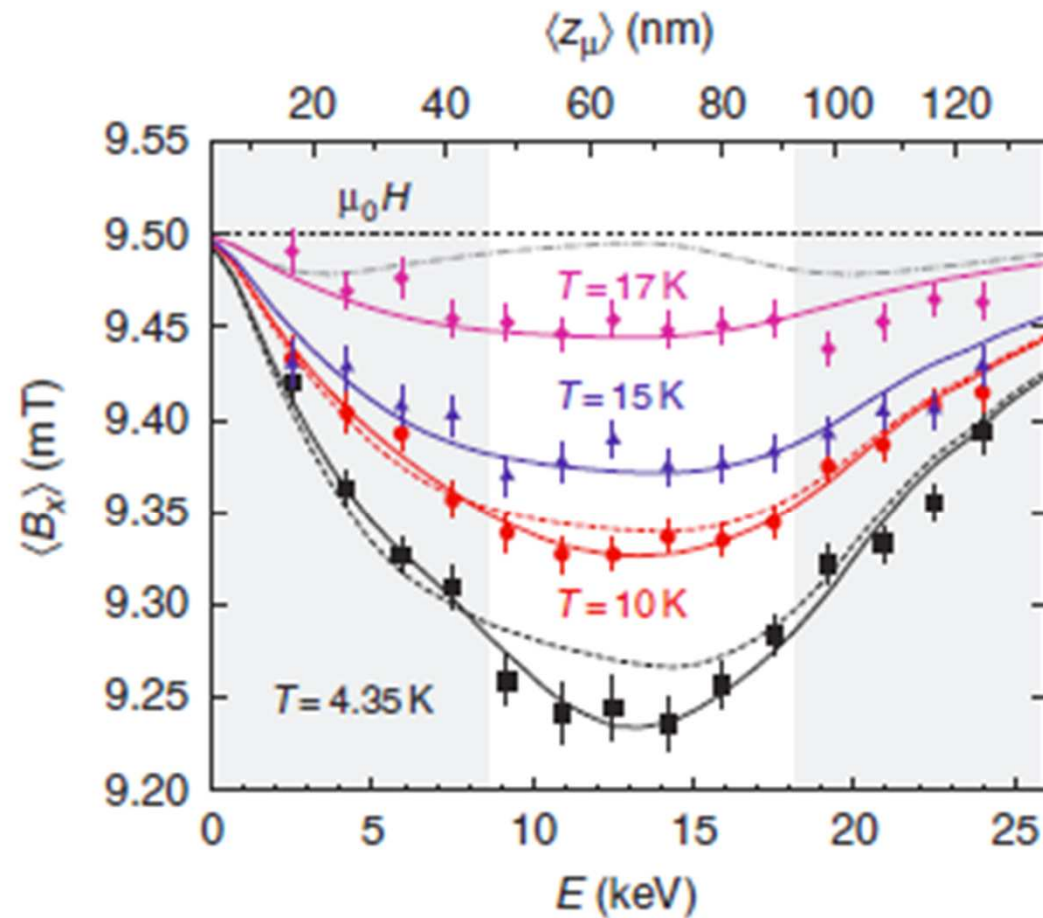


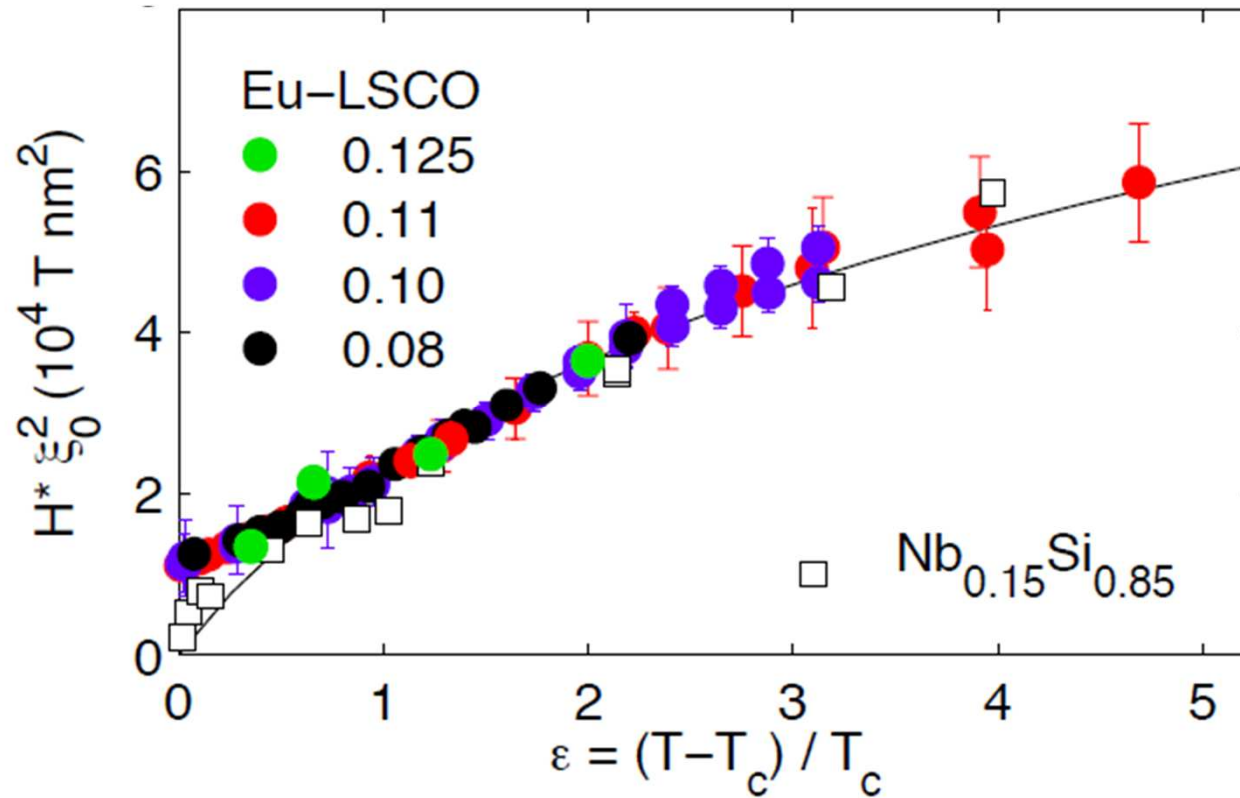
Figure 6 | Depth profile of the local field at different temperatures. The

# Actual $T_c$ in underdoped

- Quantum and classical phase fluctuations
  - V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. **74**, 3253 (1995).
  - V. J. Emery and S. A. Kivelson, Nature **374**, 474 (1995).
  - D. Podolsky, S. Raghu, and A. Vishwanath, Phys. Rev. Lett. **99**, 117004 (2007).
  - Z. Tesanovic, Nat Phys **4**, 408 (2008).
- Magnitude fluctuations
  - I. Ussishkin, S. L. Sondhi, and D. A. Huse, Phys. Rev. Lett. **89**, 287001 (2002).
- Competing order
  - E. Fradkin, S. A. Kivelson, M. J. Lawler, J. P. Eisenstein, and A. P. Mackenzie, Annual Review of Condensed Matter Physics **1**, 153 (2010).
- Disorder
  - F. Rullier-Albenque, H. Alloul, F. Balakirev, and C. Proust, EPL (Europhysics Letters) **81**, 37008 (2008).
  - H. Alloul, J. Bobro, M. Gabay, and P. J. Hirschfeld, Rev. Mod. Phys. **81**, 45 (2009).



# Gaussian amplitude fluctuations in Eu-LSCO

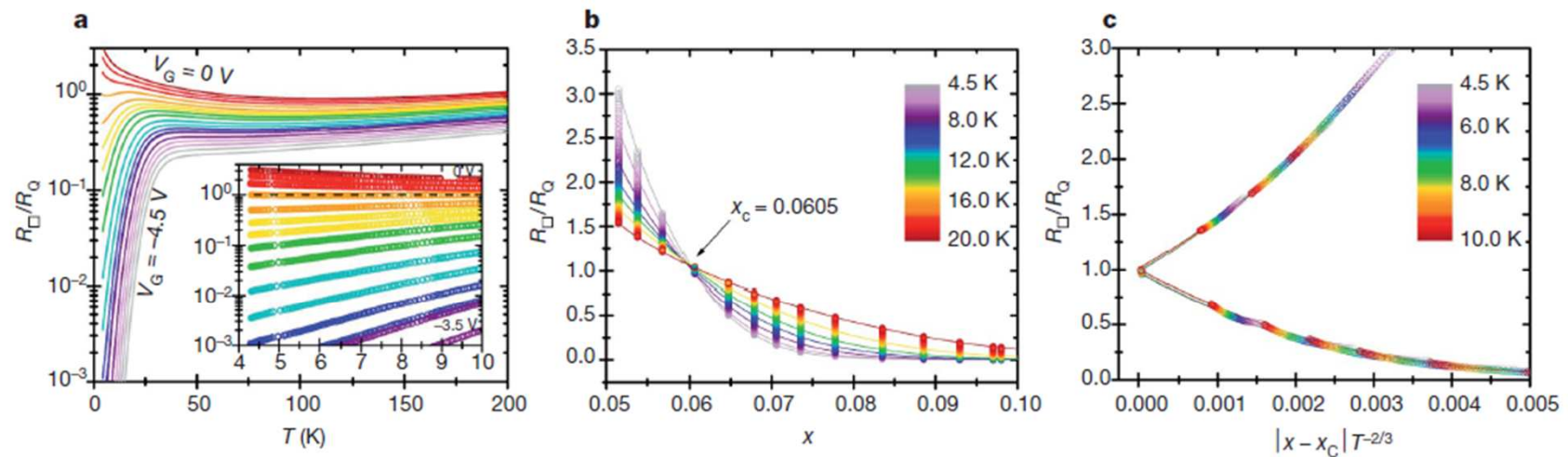


Chang, Doiron-Leyraud et al.

# Phase fluctuations and disorder?

## Monolayer LSCO, field doped

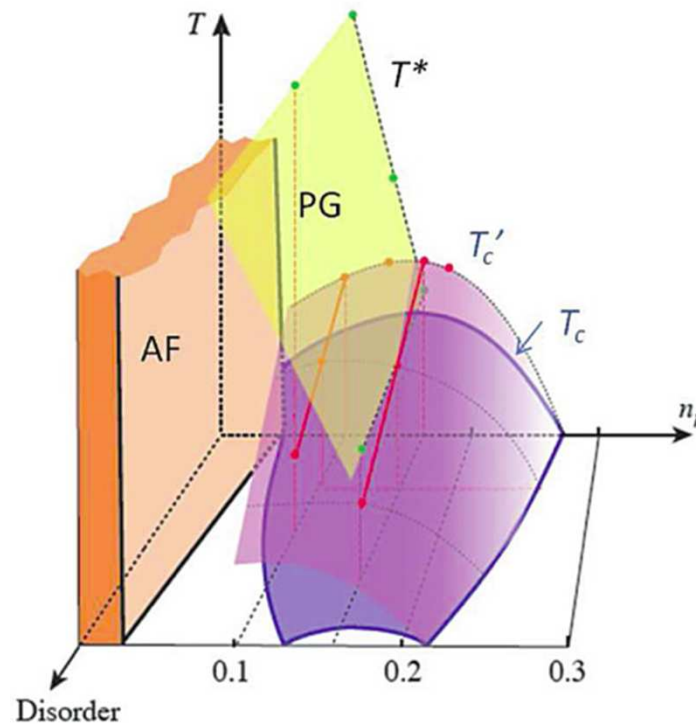
A. T. Bollinger et al. & I. Božović, *Nature* **472**, 458–460



**Figure 2 | Superconductor–insulator transition driven by electric field.** a, Temperature dependence of normalized resistance  $r = R_{\square}(x, T)/R_Q$  of an initially heavily underdoped and insulating film (see Supplementary Fig. 12 for linear scale). The device (Supplementary section B) employs a coplanar Au gate and DEME-TFSI ionic liquid. The carrier density, fixed for each curve, is tuned by varying the gate voltage from 0 V to  $-4.5$  V in 0.25 V steps; an insulating film becomes superconducting via a QPT. The inset highlights a separatrix independent of temperature below 10 K. The open circles are the actual raw data points; the black dashed line is  $R_{\square}(x_c, T) = R_Q = 6.45$  k $\Omega$ . b, The inverse representation of the same data, that is, the  $r_T(x)$  dependence at fixed temperatures below 20 K. Each vertical array of (about 100) data points corresponds to one fixed carrier density, that is, to one  $r_x(T)$  curve in Fig. 2a.

The colours refer to the temperature, and the continuous lines are interpolated for selected temperatures (4.5, 6.0, 8.0, 10.0, 12.0, 15.0 and 20.0 K). The crossing point defines the critical carrier concentration  $x_c = 0.06 \pm 0.01$ , and the critical resistance  $R_c = 6.45 \pm 0.10$  k $\Omega$ . c, Scaling of the same data with respect to a single variable  $u = |x - x_c| T^{-1/zv}$ , with  $zv = 1.5$ . This figure is derived by folding panel b at  $x_c$  and scaling the abscissa of each  $r_T(|x - x_c|)$  curve by  $T^{-2/3}$ . For  $4.3$  K  $< T < 10$  K, the discrete groups of points of Fig. 2b collapse accurately onto a two-valued function, with one branch corresponding to  $x$  larger and the other to  $x$  smaller than  $x_c$ . The critical exponents are identical on both sides of the superconductor–insulator transition. The raw data points cover the interpolation lines almost completely, except close to the origin.

# Effect of disorder

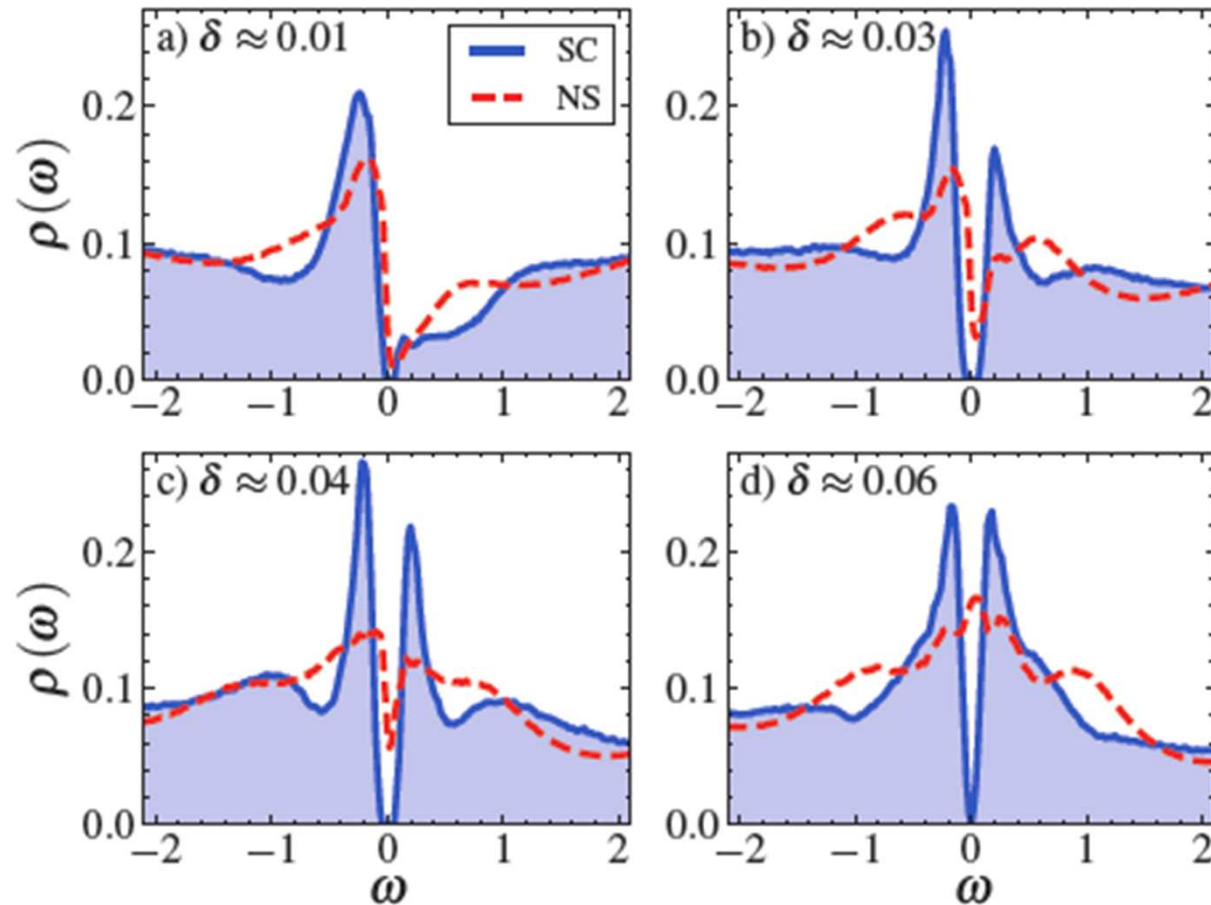


F. Rullier-Albenque, H. Alloul, and G. Rikken,  
Phys. Rev. B **84**, 014522 (2011).

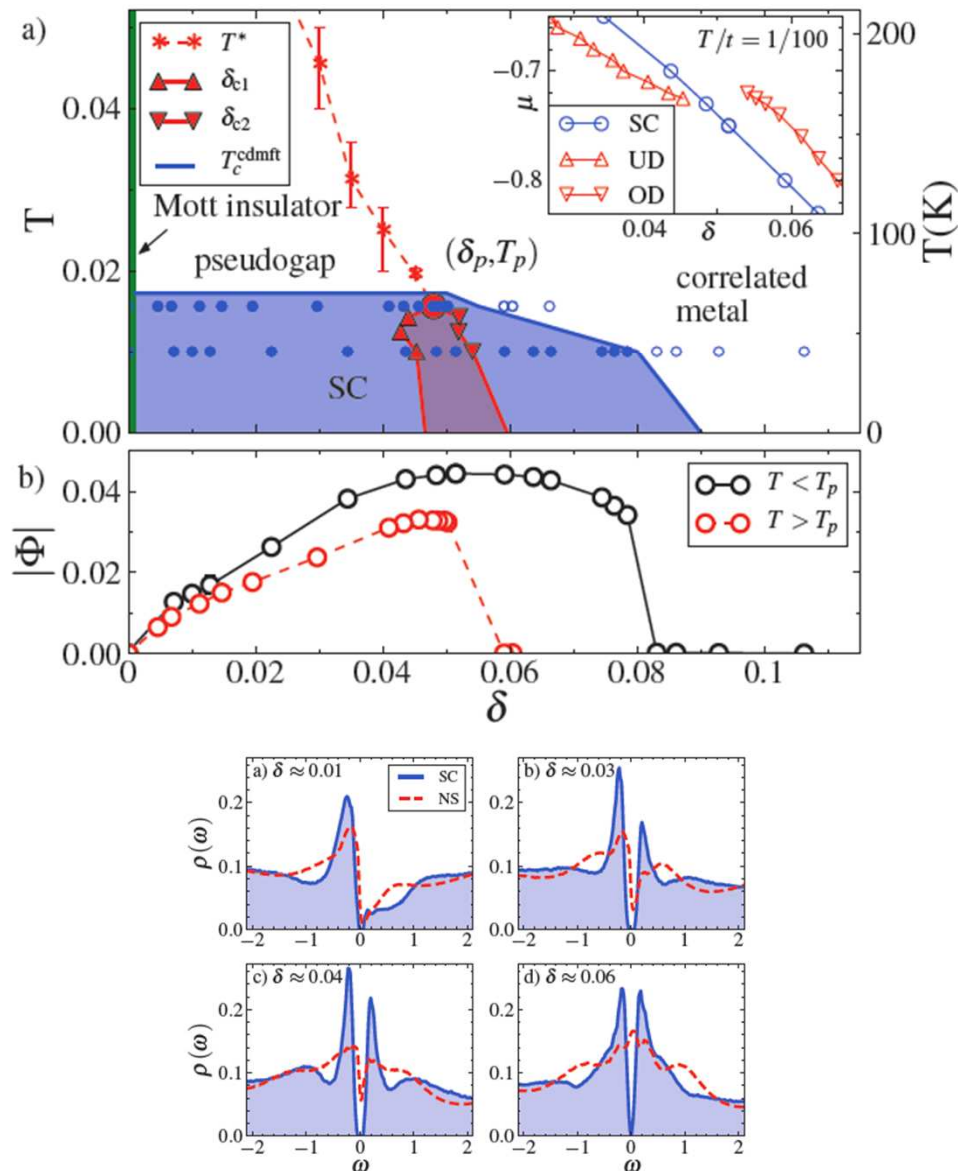
# Superconductivity in underdoped vs BCS



# First-order transition leaves its mark

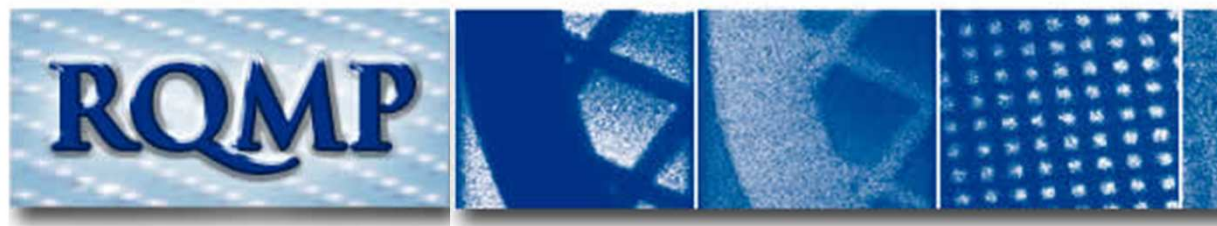
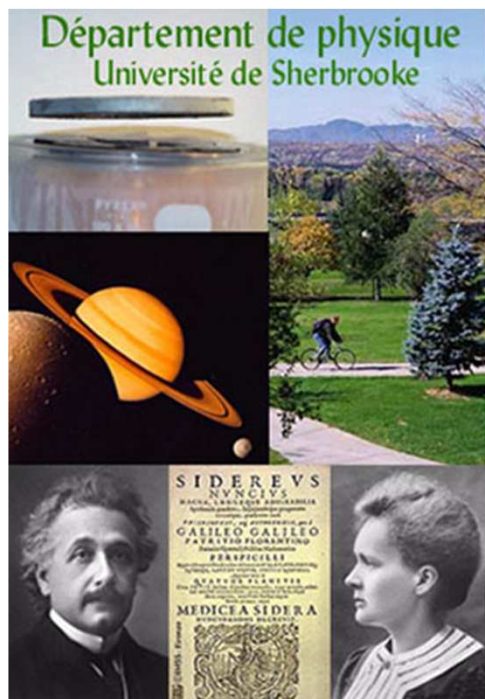


# Summary



- Below the dome finite  $T$  critical point (not QCP) controls normal state
- First-order transition destroyed but traces in the dynamics
- Pseudogap different from pairing.
- Actual  $T_c$  in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder

# André-Marie Tremblay



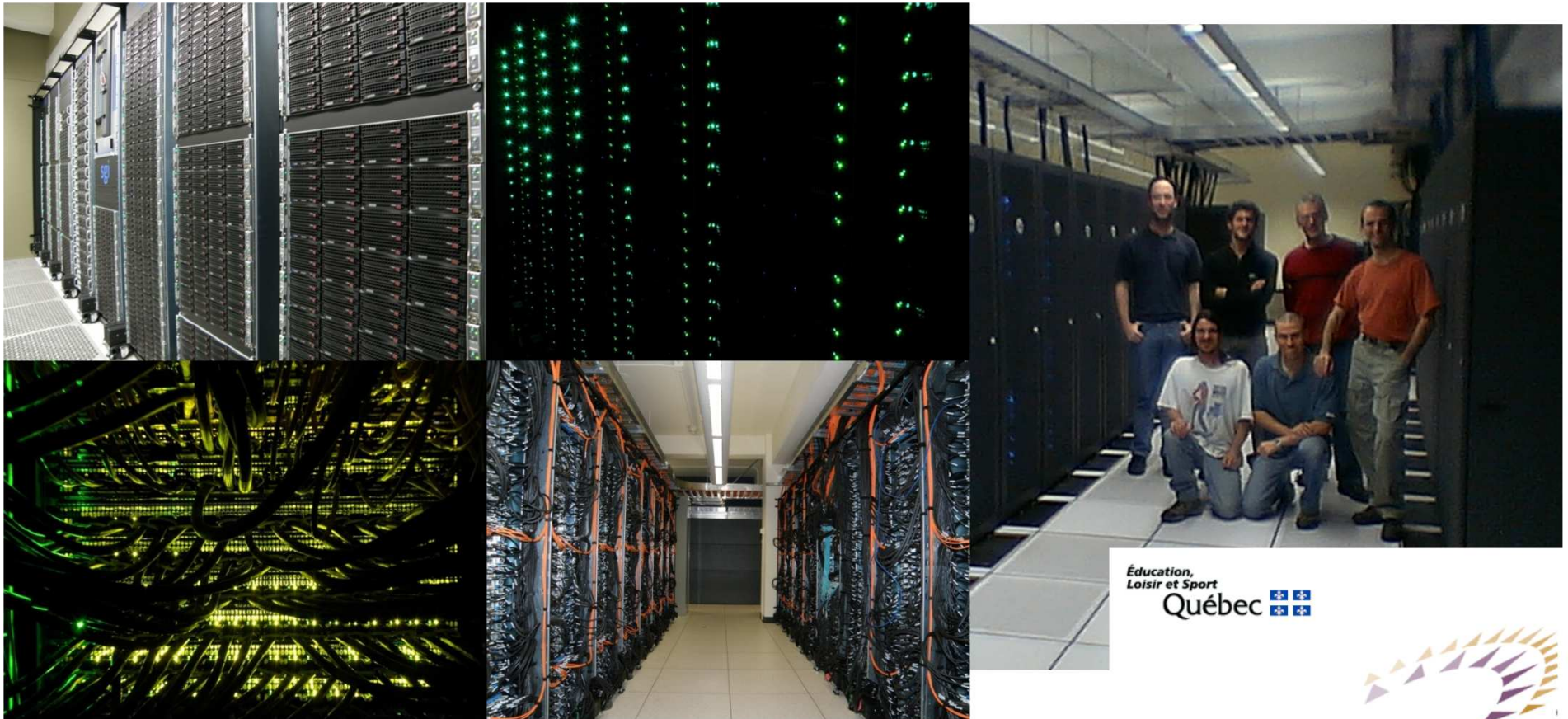
Le regroupement québécois sur les matériaux de pointe



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DRIVING INNOVATION  
BUILDING THE DIGITAL ECONOMY

**Le calcul de haute performance**

CRÉER LE SAVOIR  
ALIMENTER L'INNOVATION  
BÂTIR L'ÉCONOMIE NUMÉRIQUE



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Merci

Thank you