

# An organizing principle for 2D strongly correlated superconductivity

**L. Fratino et al., Scientific Reports 6, 22715 (2016)**

**L. Fratino et al., Phys. Rev. B 93, 245147 (2016)**

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NGSCES, 2016



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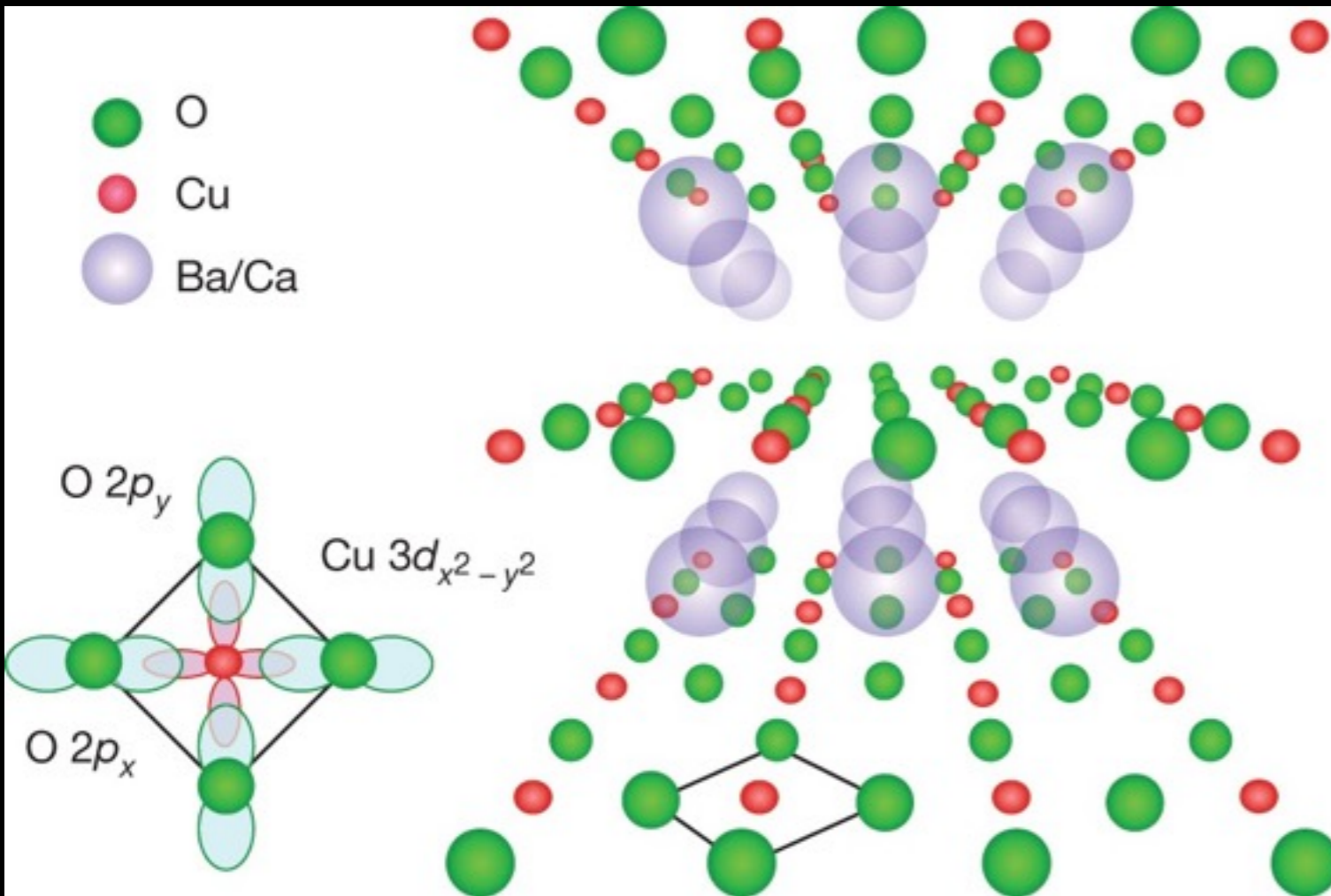
*Université de Sherbrooke  
- Rutgers university*



**André-Marie Tremblay**

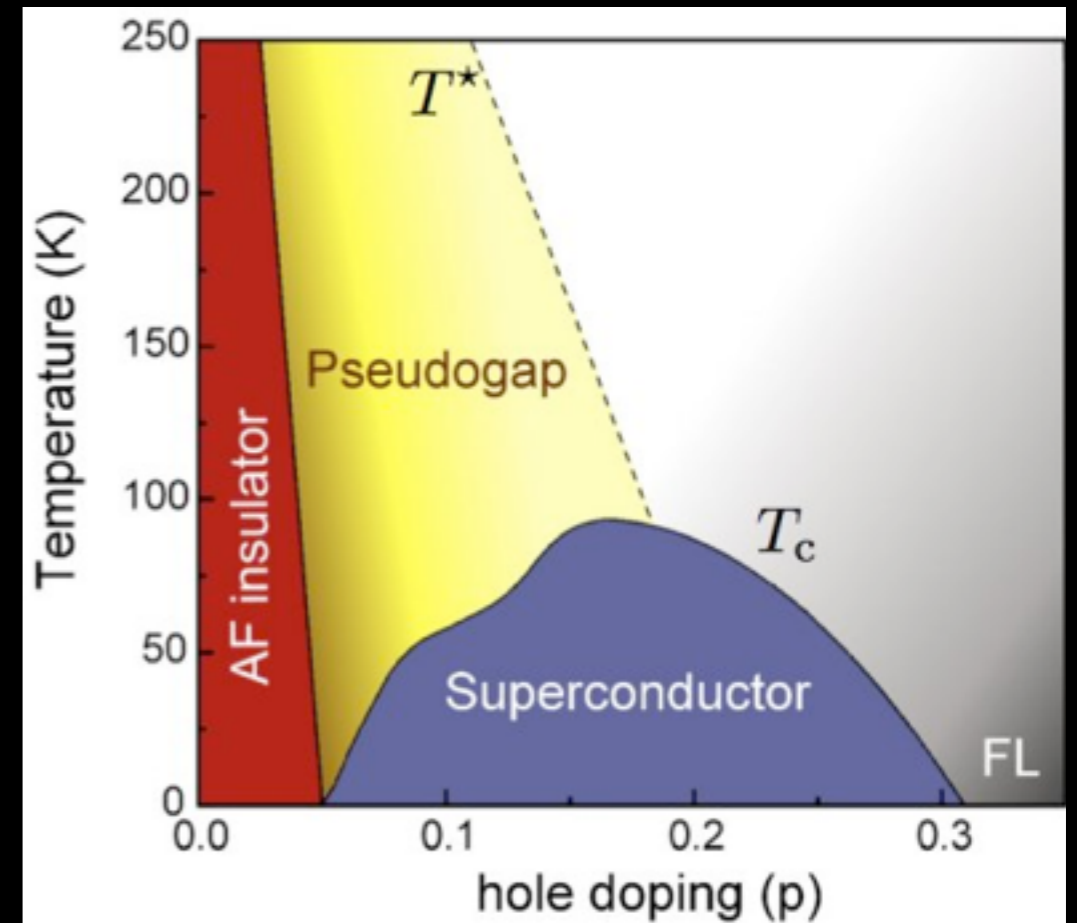
*Université de Sherbrooke*

# Cuprates



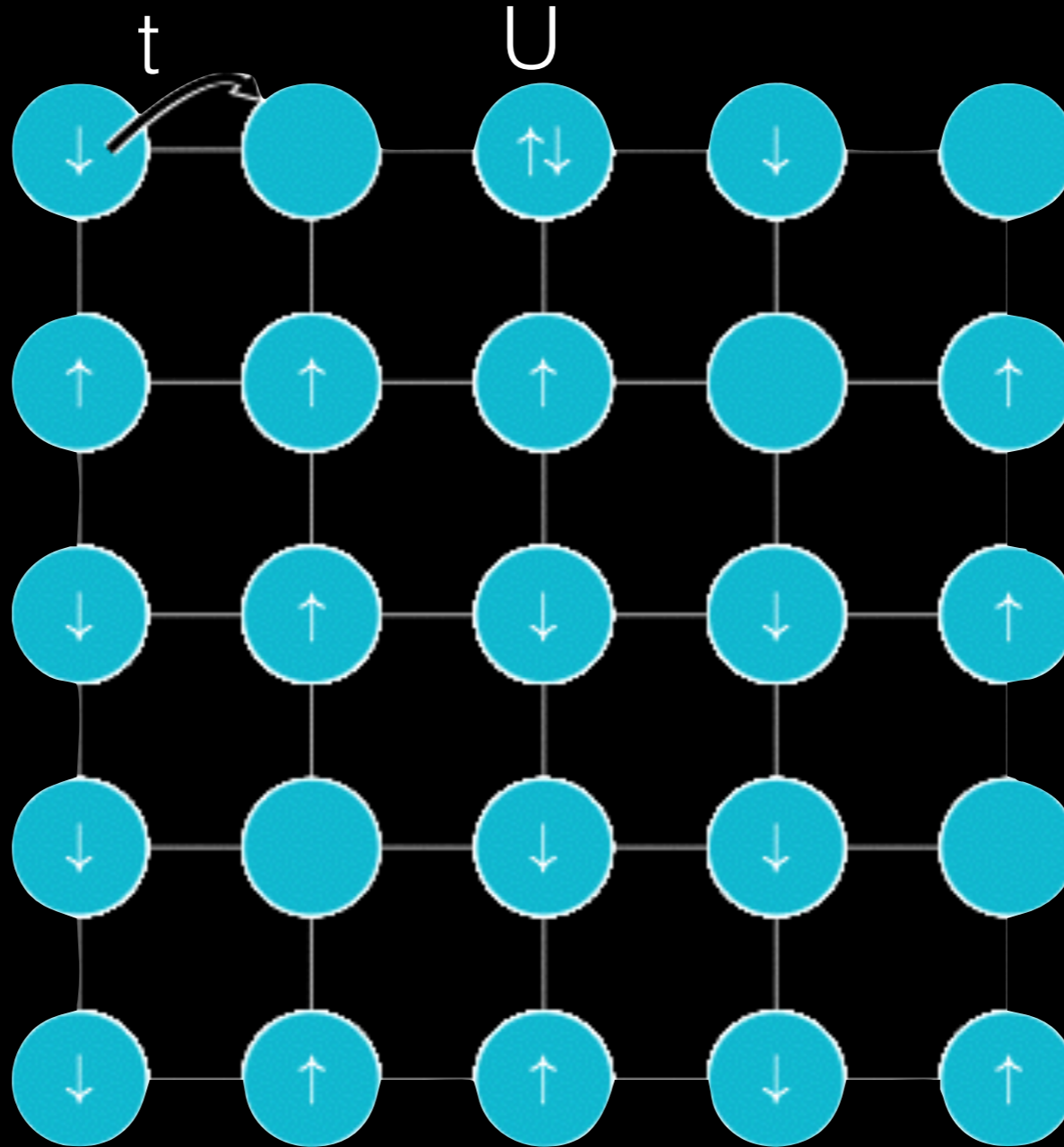
2D copper oxide layers

**Keimer B., Nat. Phys. (2015)**



Doped Mott insulators

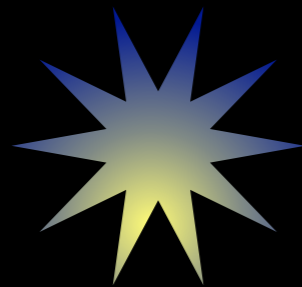
# Hubbard Model



The simplest model that can capture the essential physics of such systems is the single-band Hubbard model:

$$\hat{H}_{HM} = - \sum_{\langle i,j \rangle, \sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{\sigma, i} \hat{n}_{i\sigma}$$

# doping-driven Mott transition: 2D Hubbard model scenario



Mott insulating phase



pseudogap phase



correlated metallic phase



sharp crossovers in

- dynamic
- thermodynamic and
- transport properties



momentum differentiation



d-wave superconducting  
dome



energetics of SC



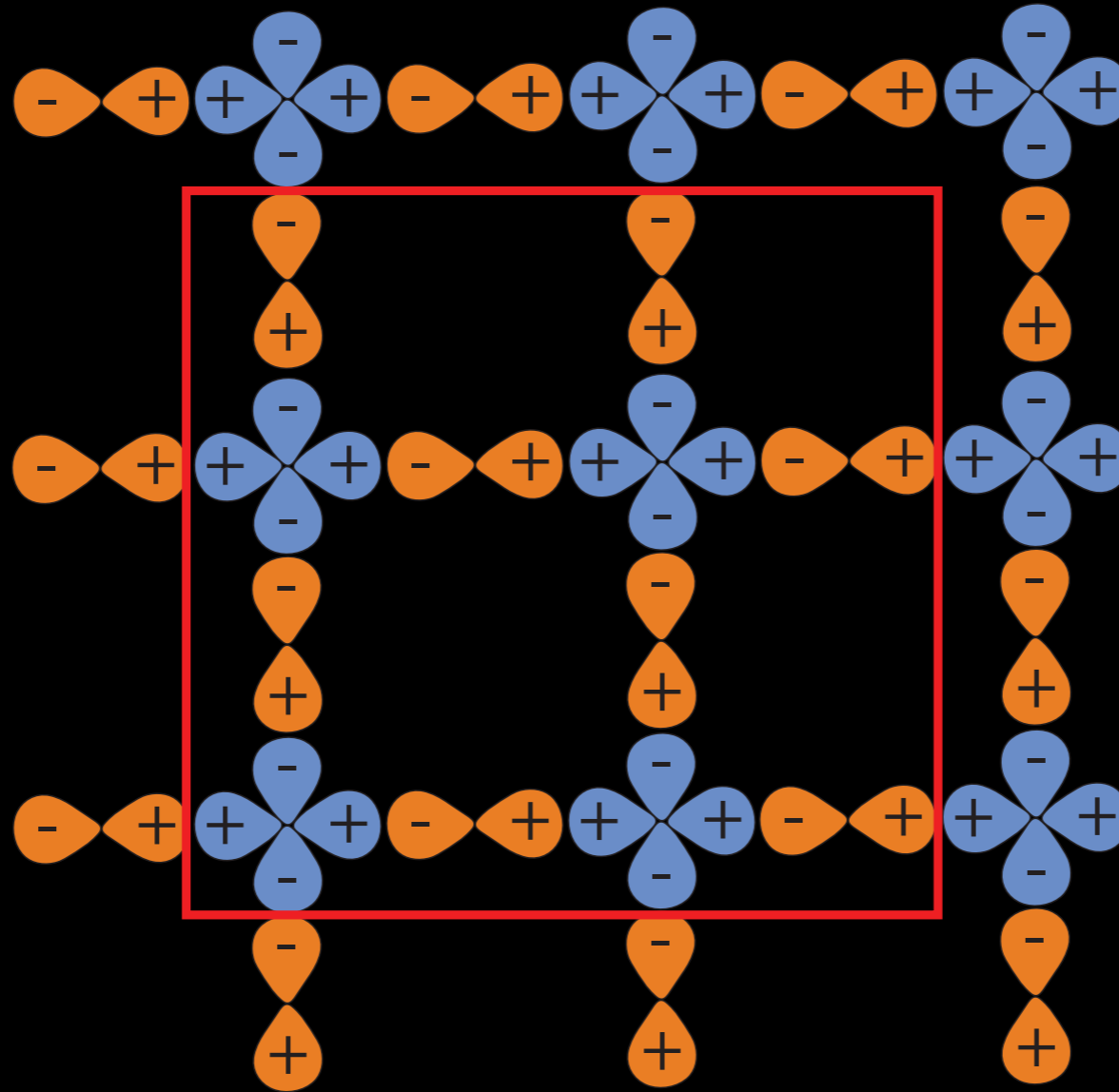
interplay Mott physics/  
pseudogap/  
superconductivity



**our contribution:**

an **organizing principle** for both  
normal and superconducting phase:  
**first-order transition at finite doping**



# three-band model



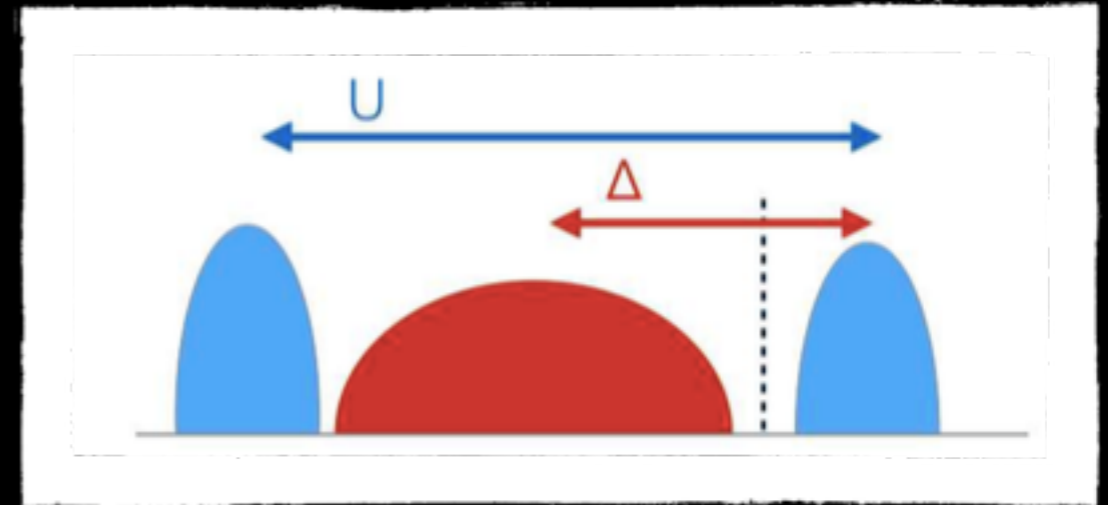
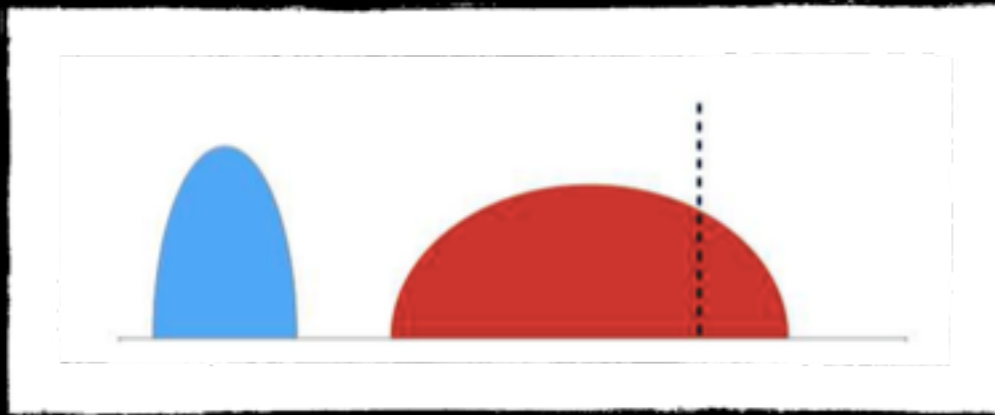
$$\mathbf{h}_0(\mathbf{k}) = \begin{pmatrix} \epsilon_d & t_{pd}(1 - e^{-ik_x}) & t_{pd}(1 - e^{-ik_y}) \\ t_{pd}(1 - e^{ik_x}) & \epsilon_p + 2t_{pp}(\cos k_x - 1) & t_{pp}(1 - e^{ik_x})(1 - e^{-ik_y}) \\ t_{pd}(1 - e^{ik_y}) & t_{pp}(1 - e^{-ik_x})(1 - e^{ik_y}) & \epsilon_p + 2t_{pp}(\cos k_y - 1) \end{pmatrix}$$

# Zaanen-Sawatzky-Allen scheme

## Charge transfer insulators

 Cu  O

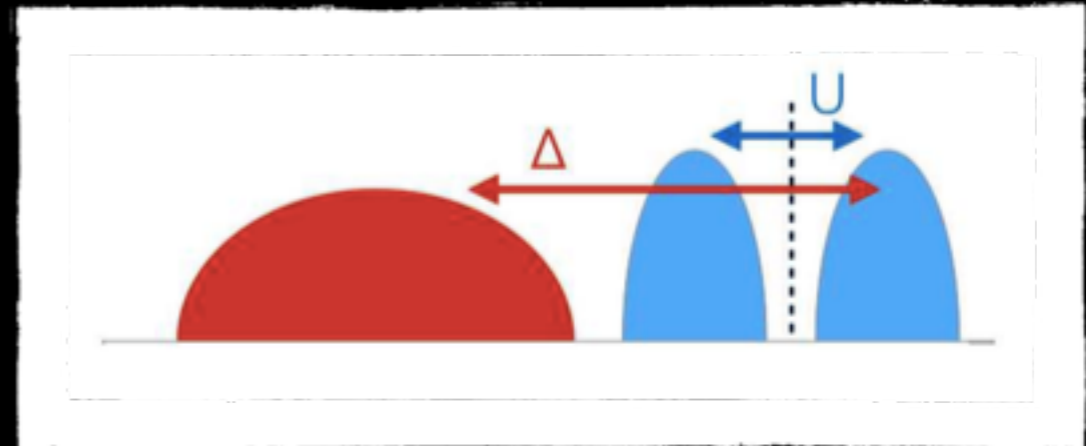
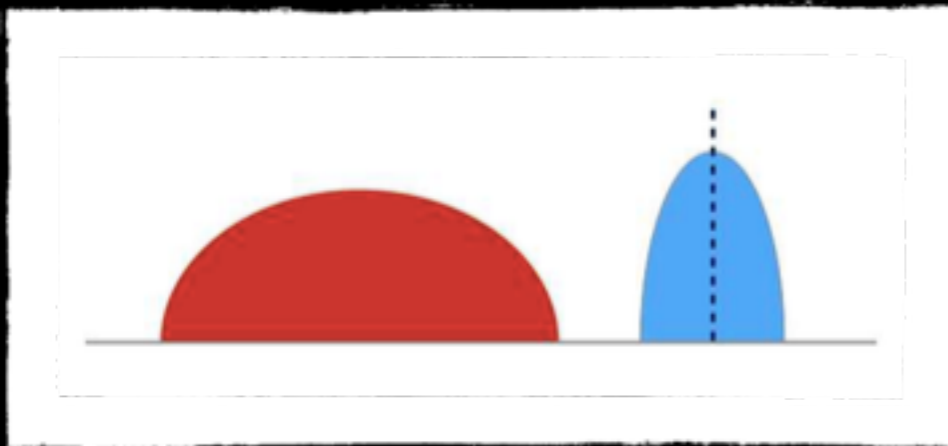
DOS



charge-transfer gap expected at  $n_{\text{tot}}=n_d+2n_p=5$

## Mott-Hubbard insulators

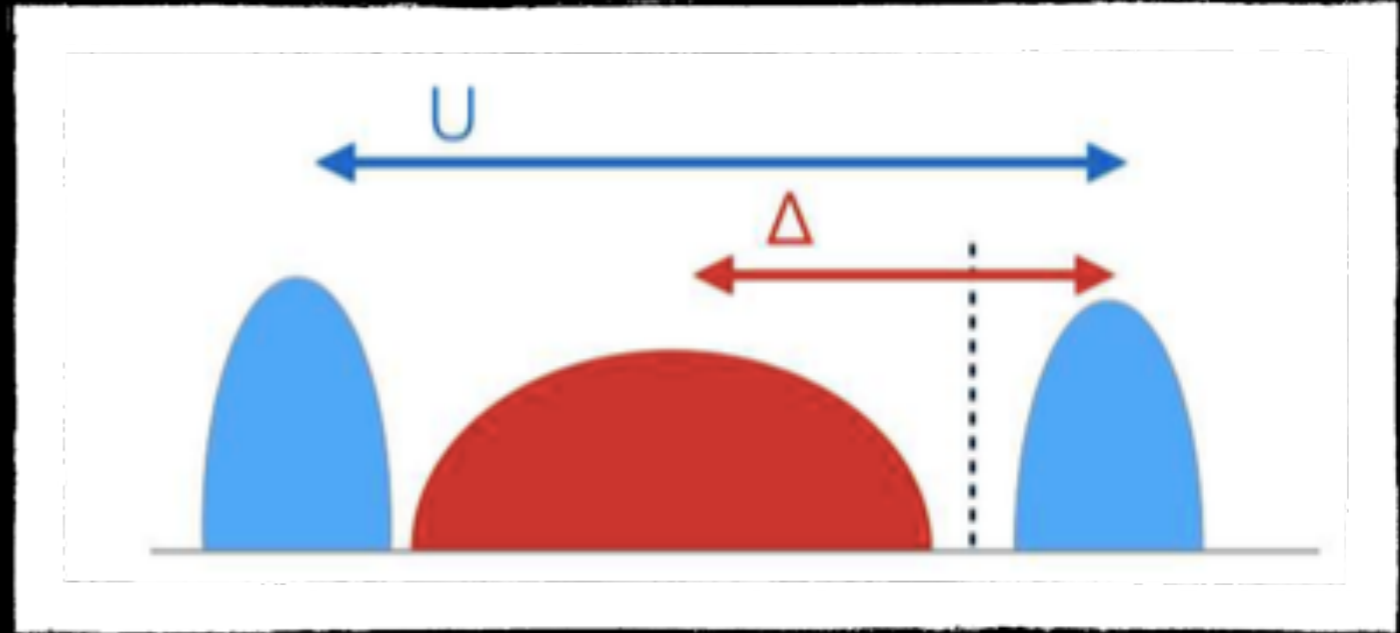
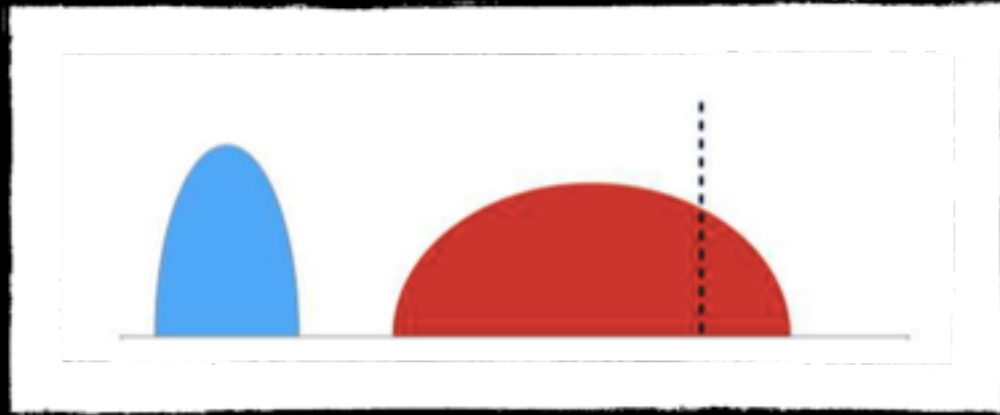
DOS



Mott-Hubbard gap expected at  $n_{\text{tot}}=n_d+2n_p=5$

# Charge transfer insulators

DOS



charge-transfer gap  
expected at  $n_{\text{tot}}=n_d+2n_p=5$

within cellular DMFT, we explore **two routes**:

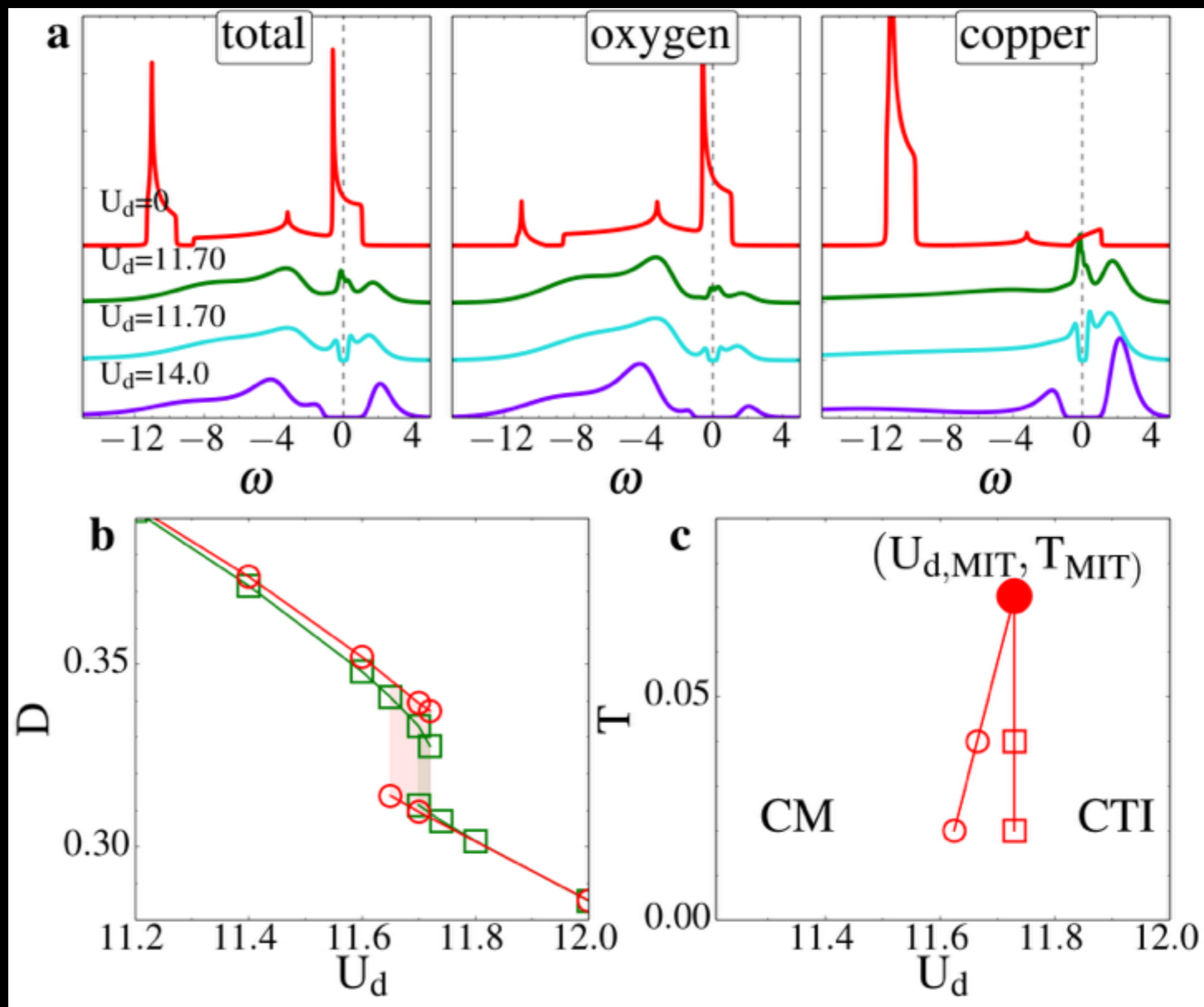
- **$U_d$  driven** metal to charge-transfer insulator transition
- **doping driven** metal to charge-transfer insulator transition



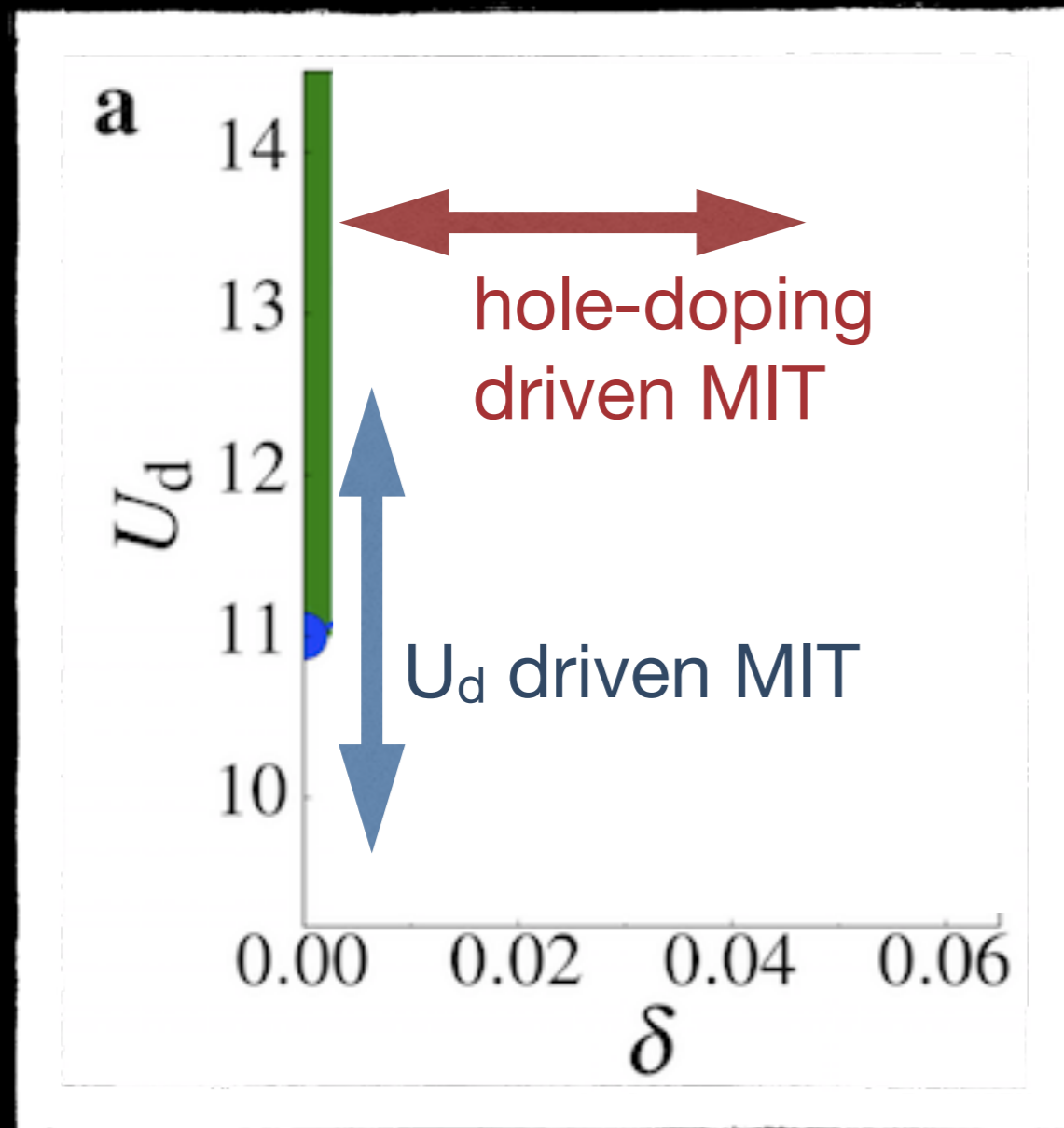
**Normal state**

**Superconducting phase**

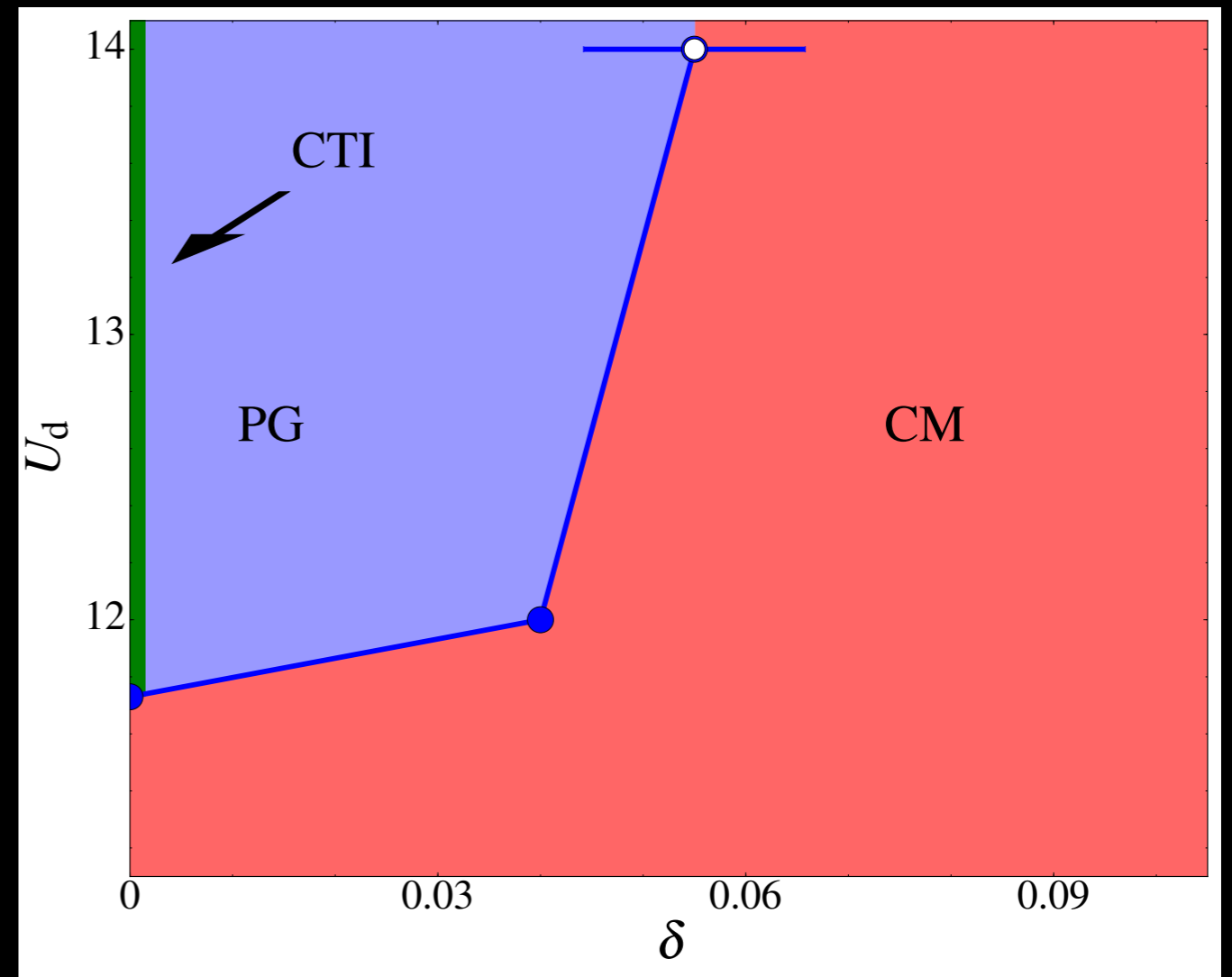
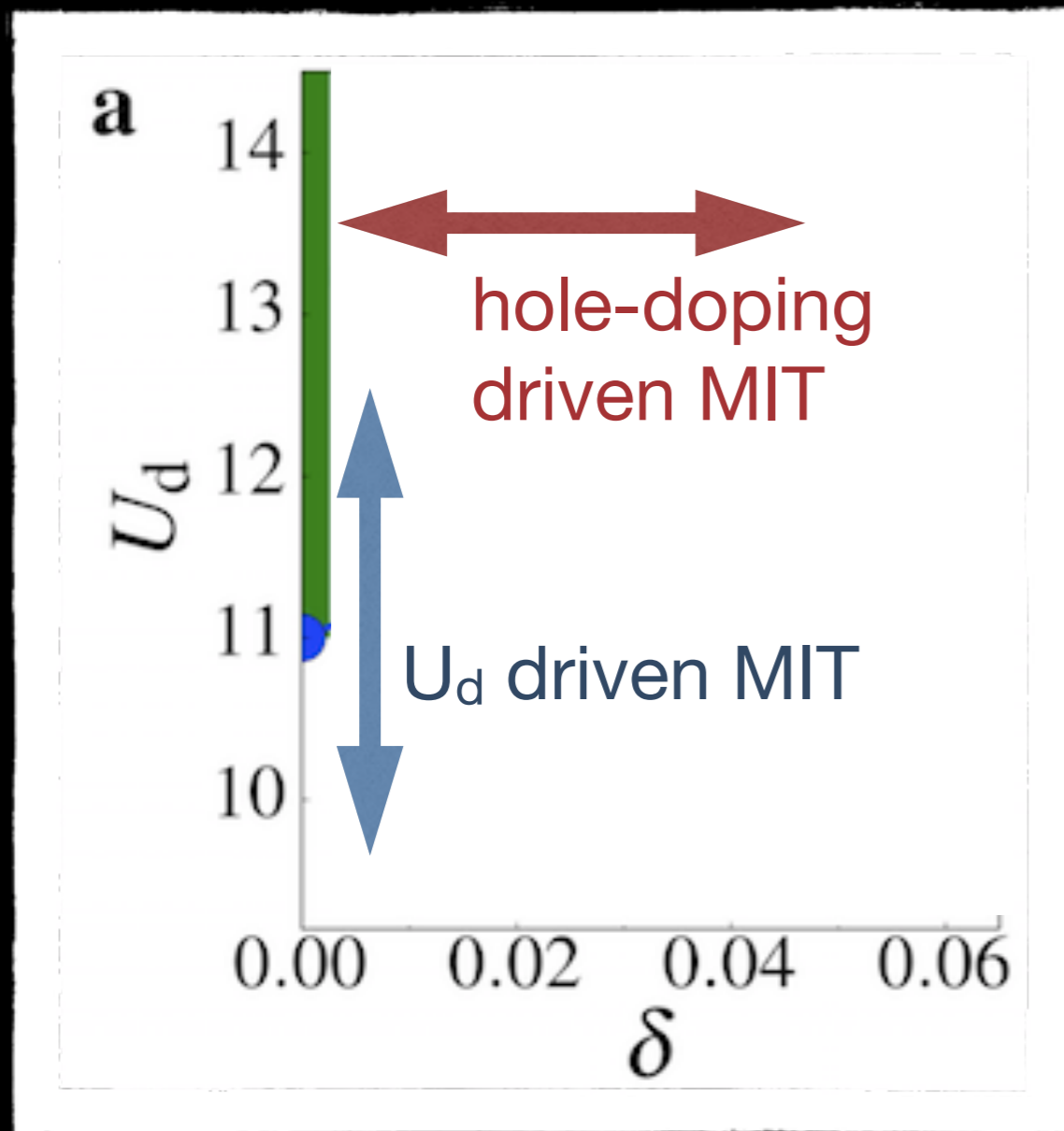
# $U_d$ driven metal-insulator transition at $n_{\text{tot}}=5$



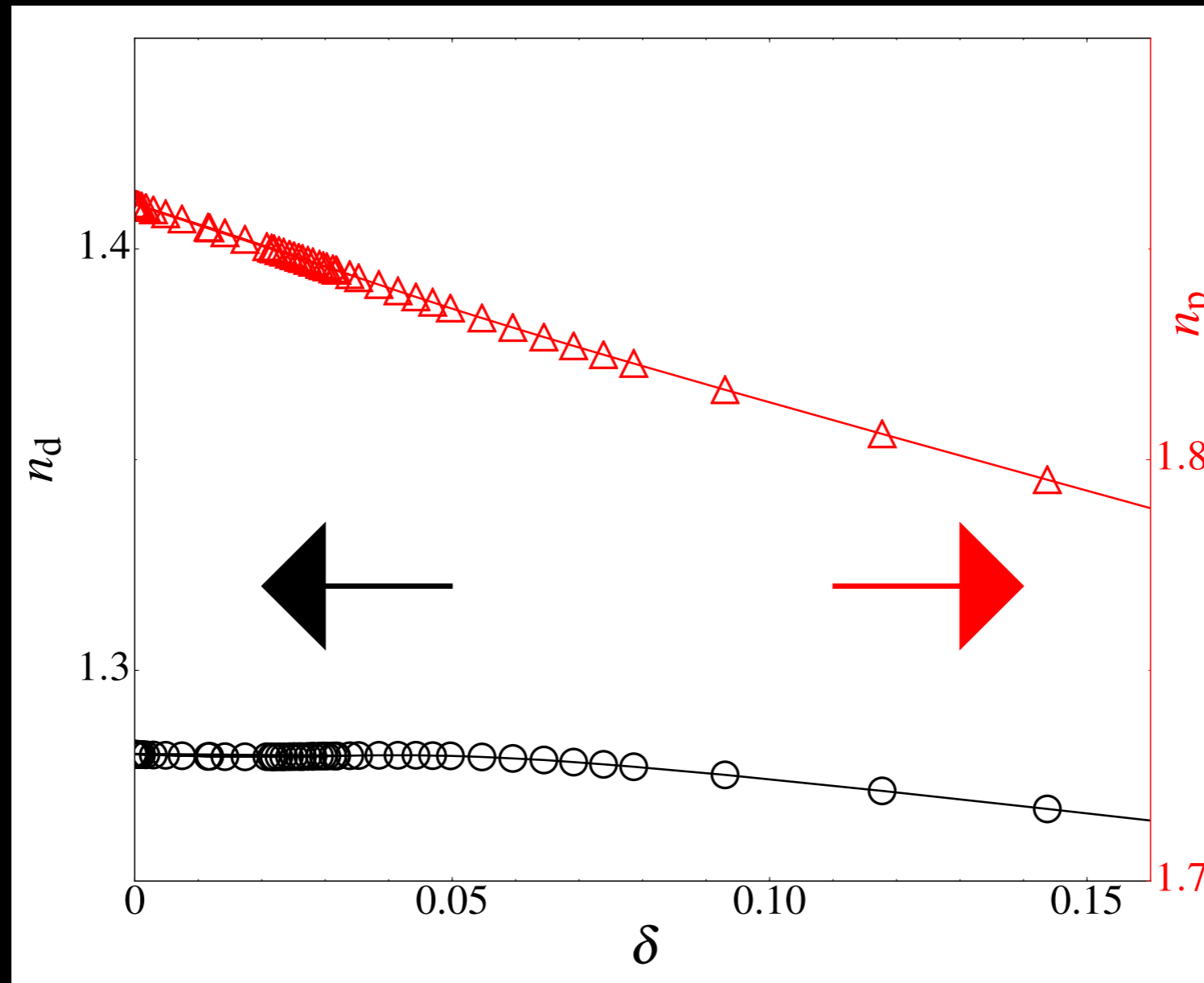
# hole-doping driven metal-insulator transition



# hole-doping driven metal-insulator transition



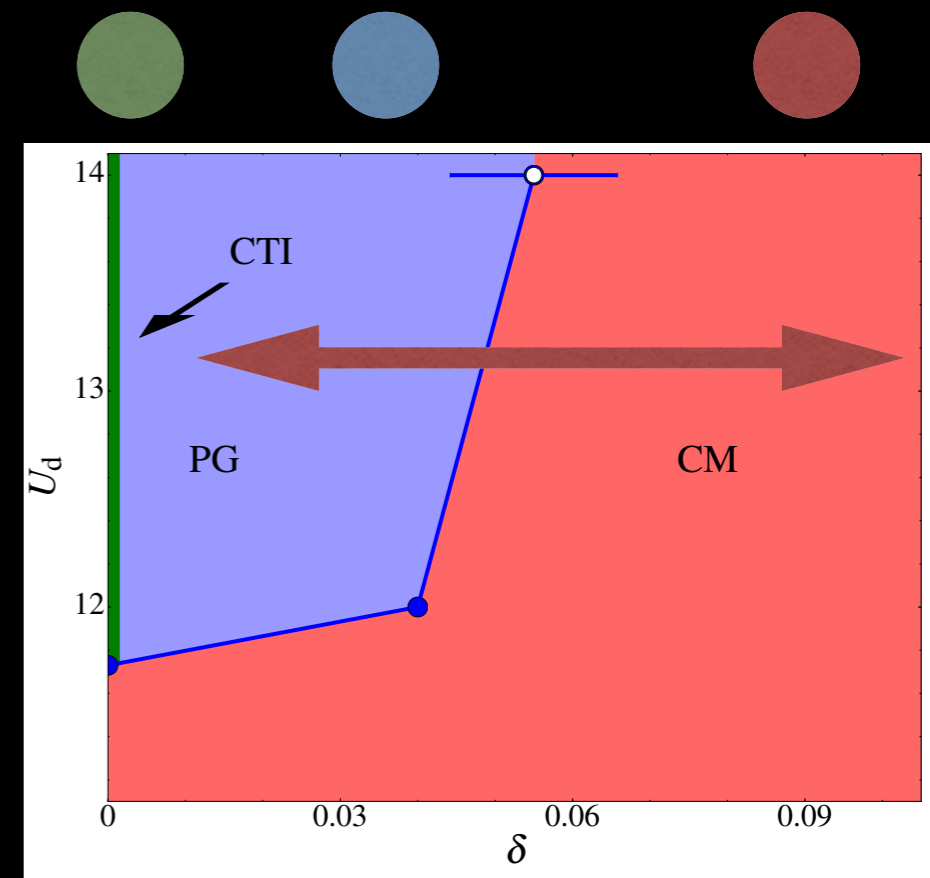
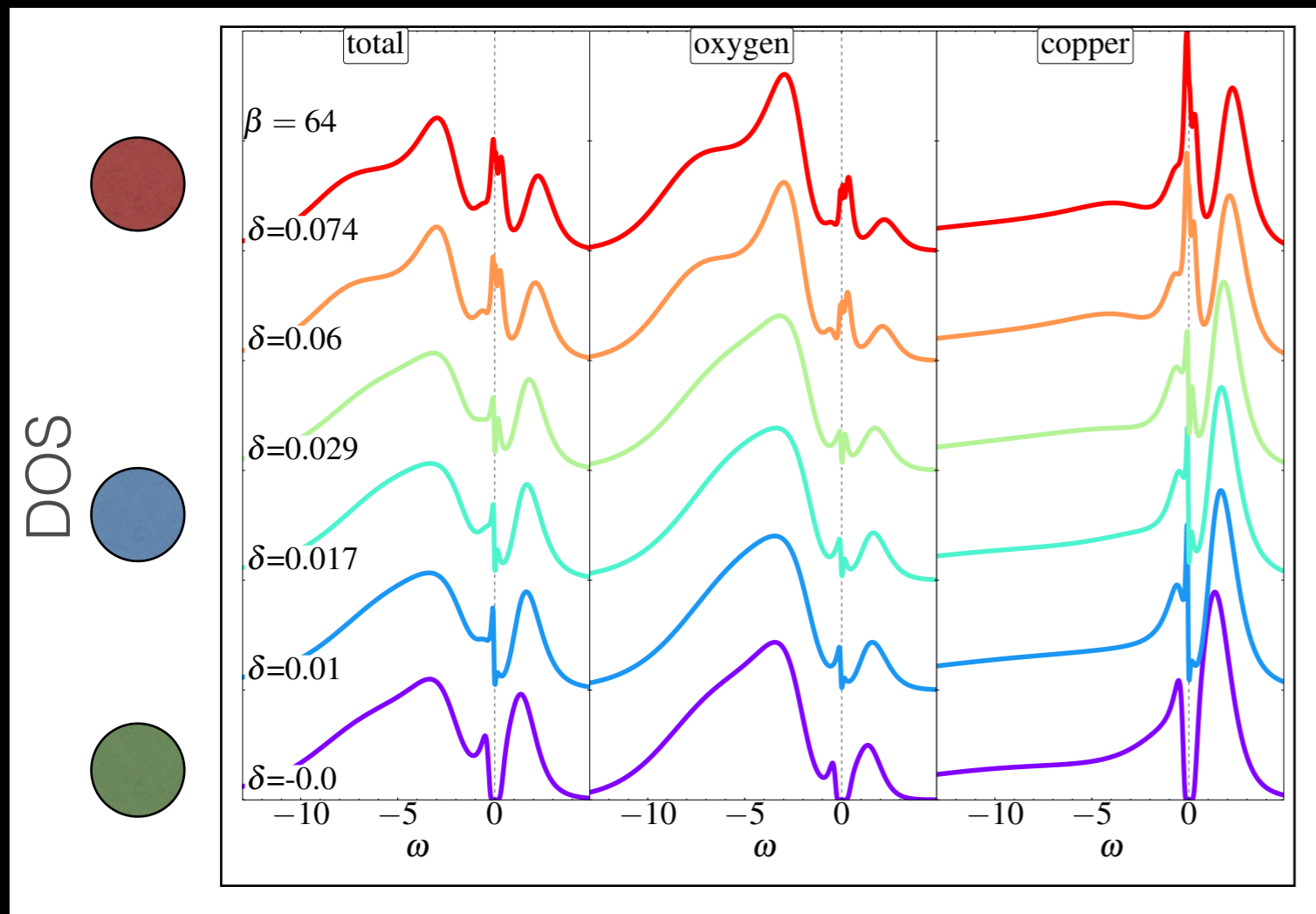
# hole-doping driven metal-insulator transition



doped holes mainly resides on oxygen

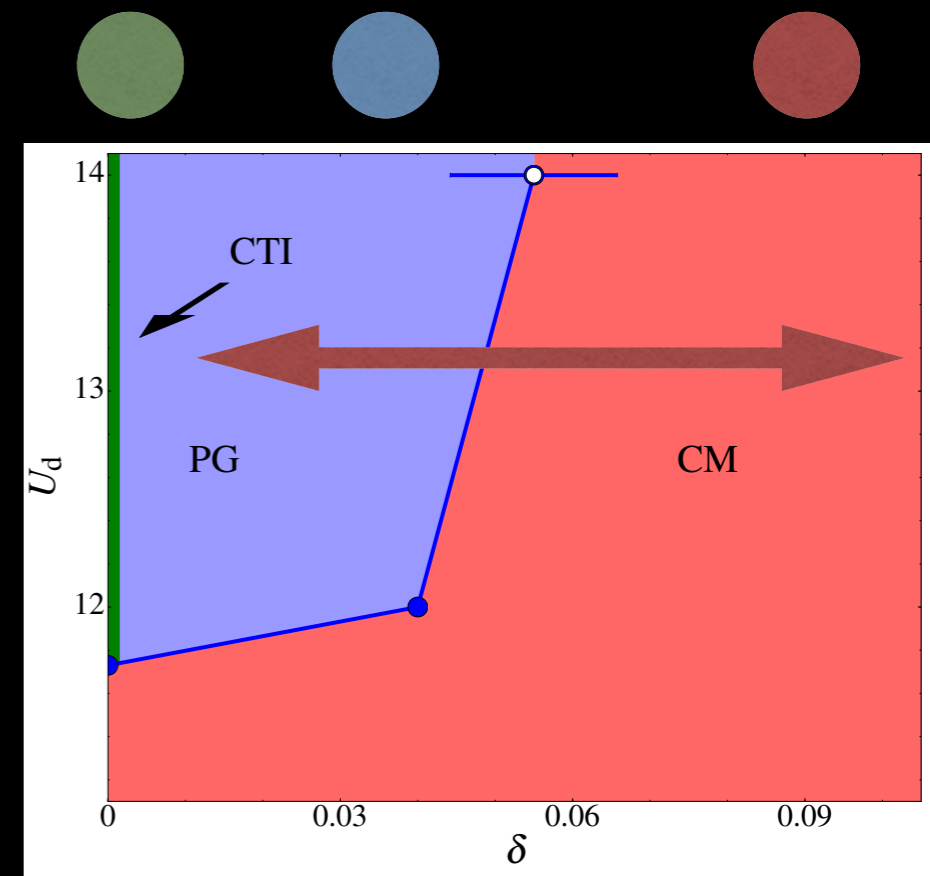
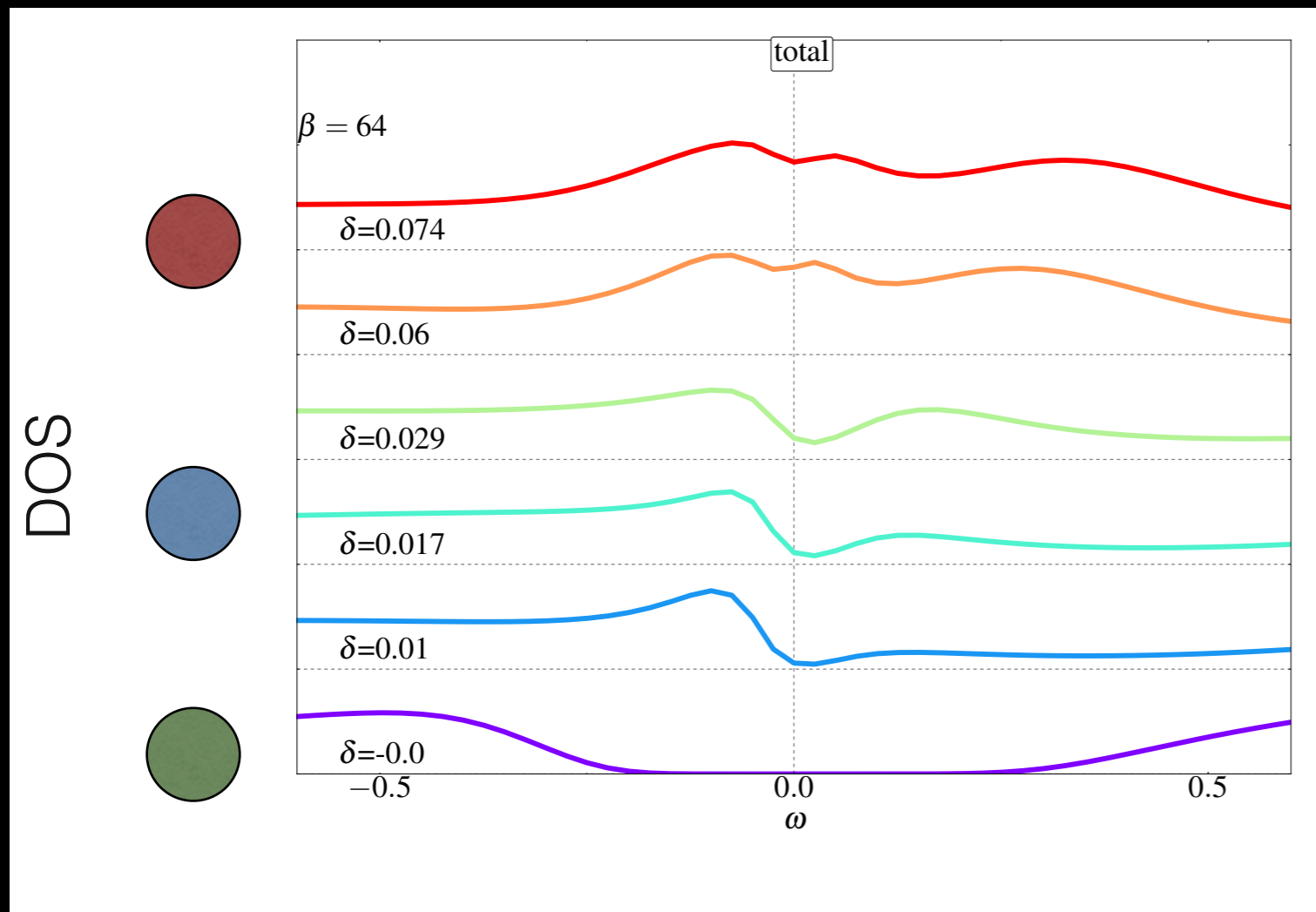
N. Gauquelin, et al., Nat. Comm. (2014)

# hole-doping driven metal-insulator transition



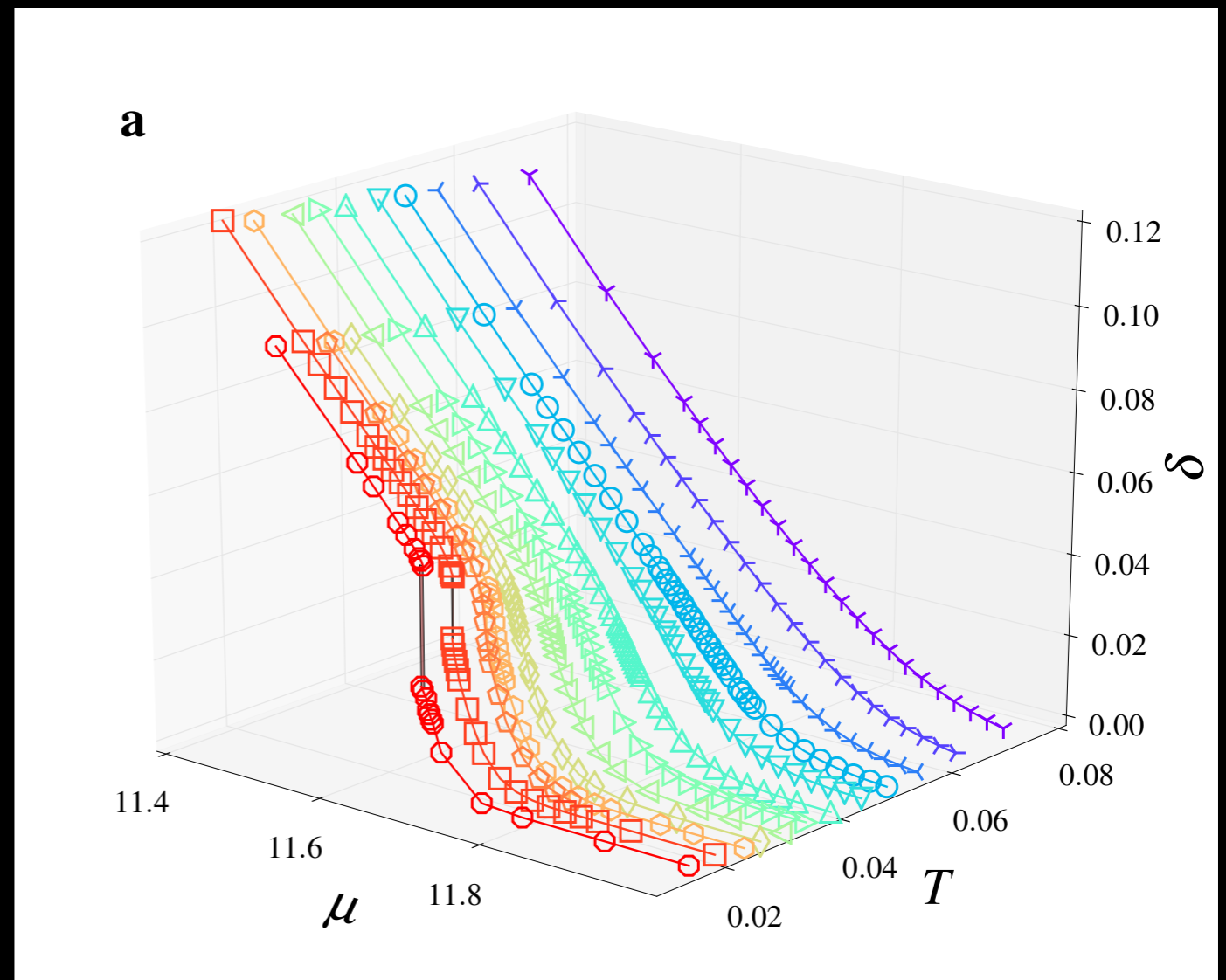
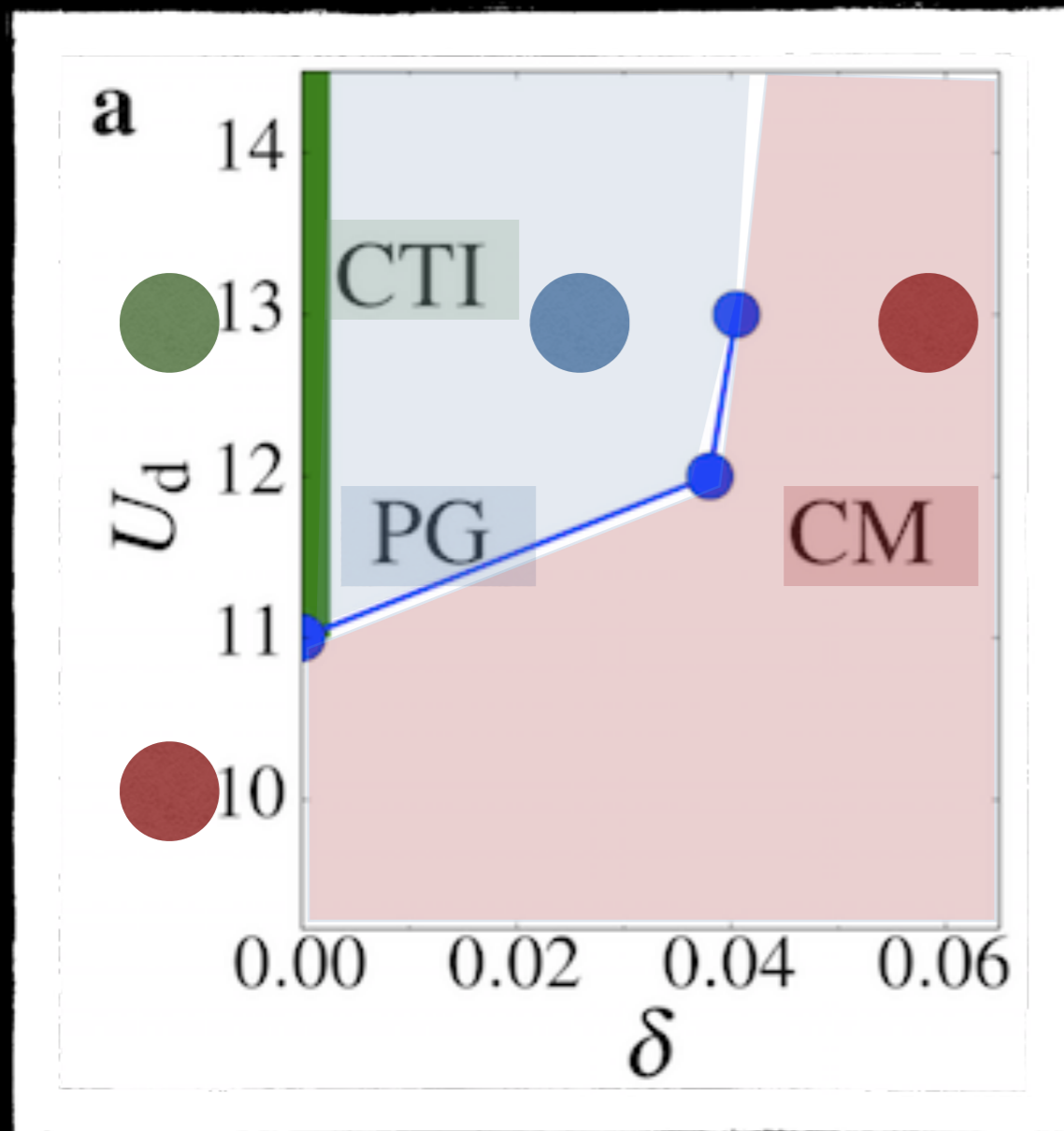
- charge-transfer-insulating phase
- pseudogap phase
- correlated metallic phase

# hole-doping driven metal-insulator transition



- charge-transfer-insulating phase
- pseudogap phase
- correlated metallic phase

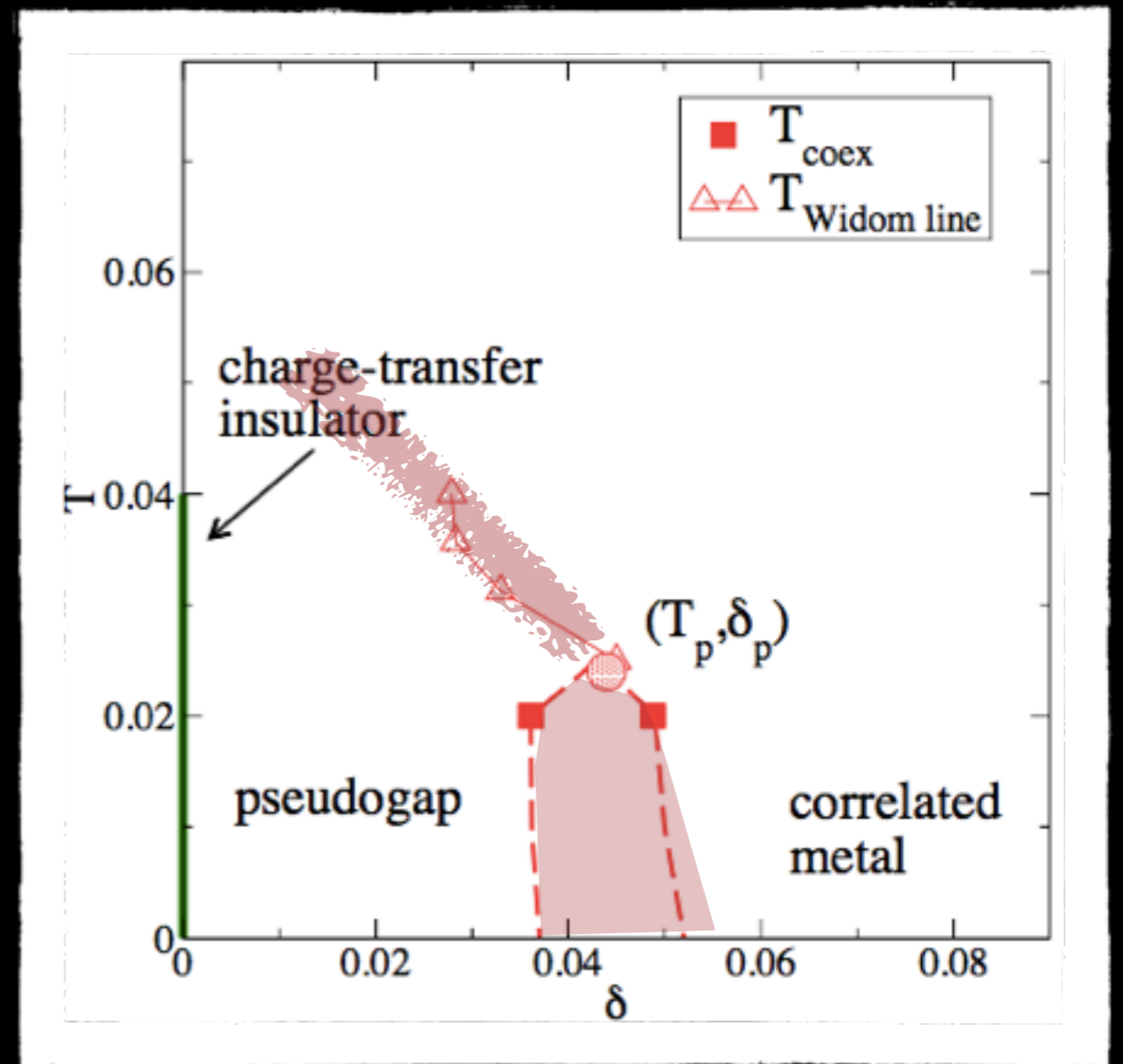
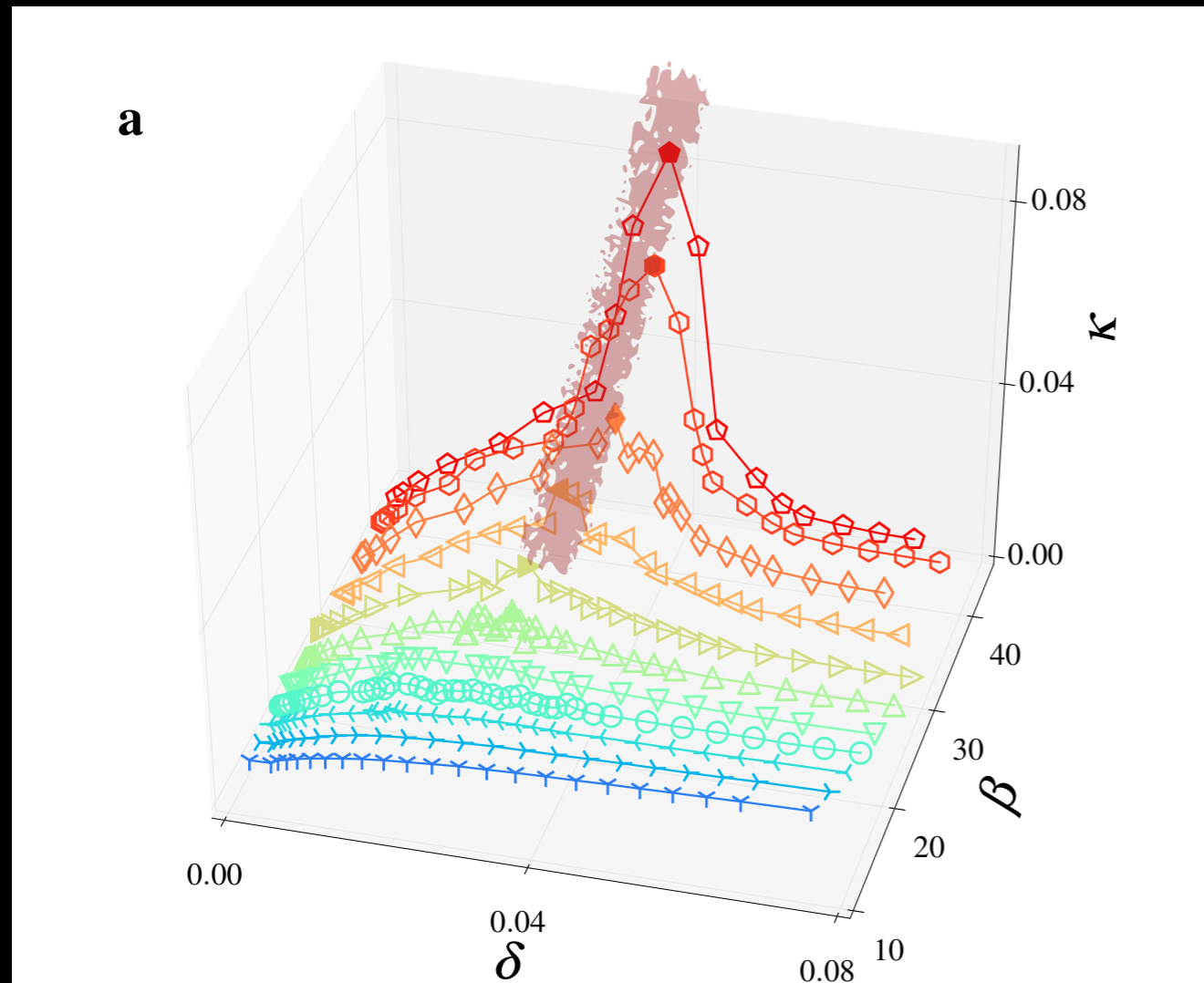
# hole-doping driven metal-insulator transition



First-order transition at finite doping between two different metals linked to Mott physics



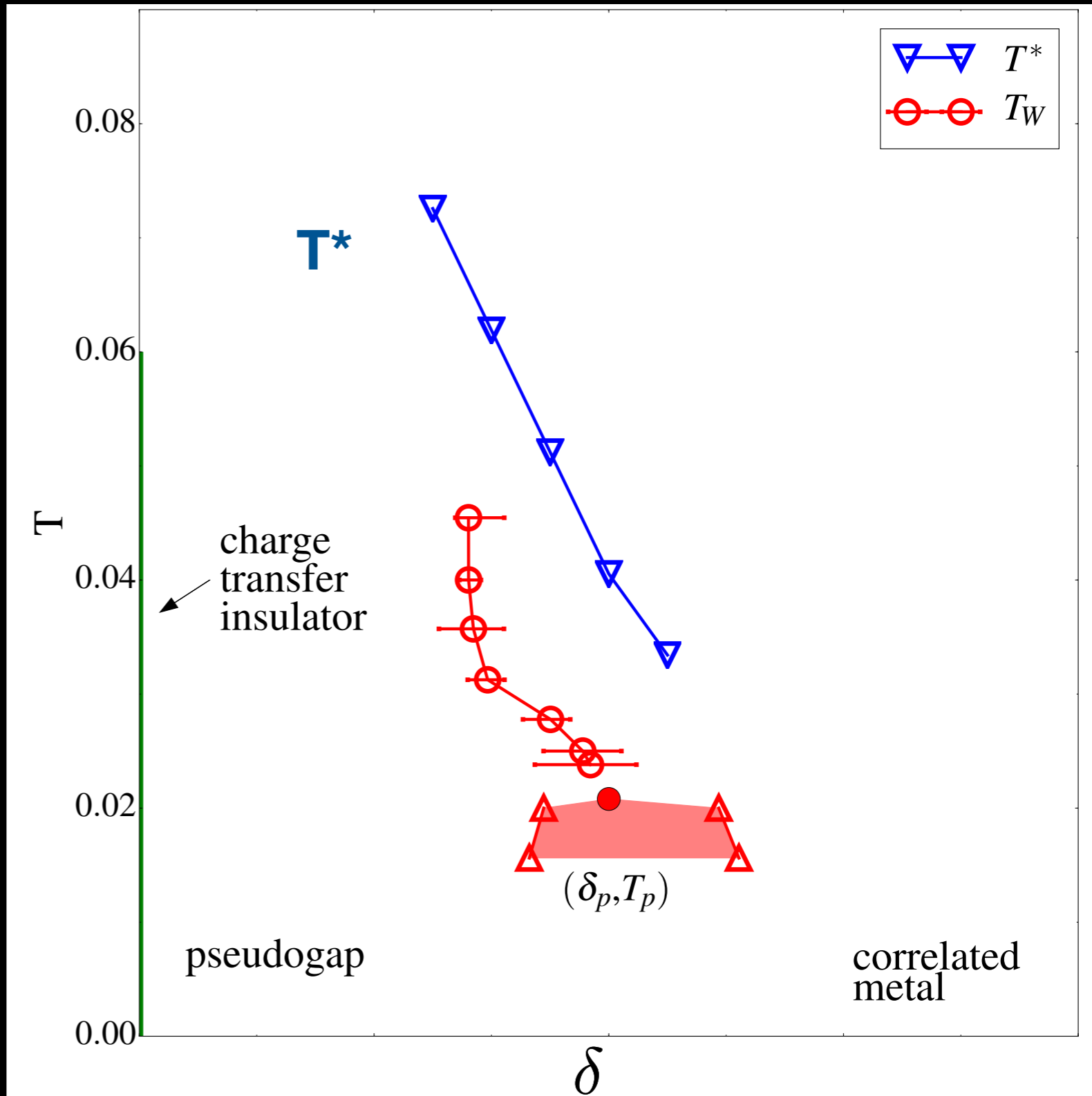
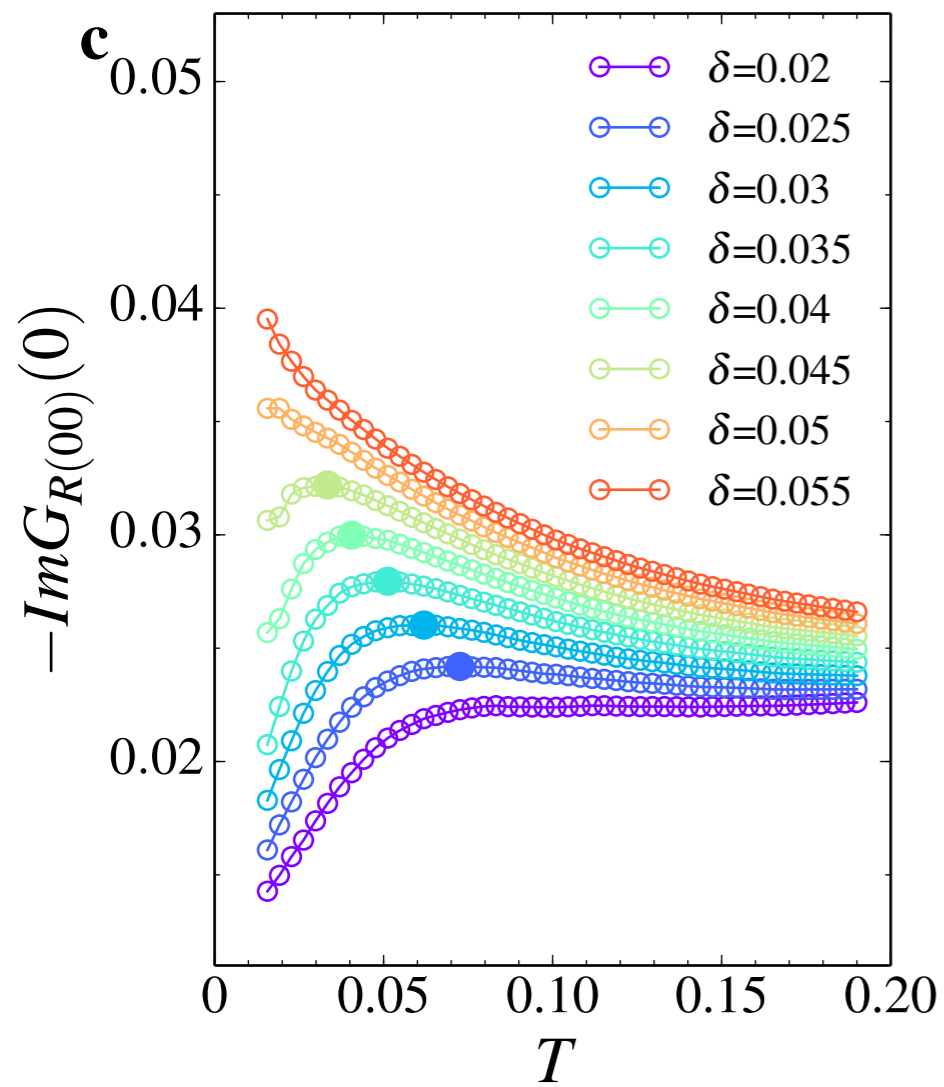
# hole-doping driven metal-insulator transition



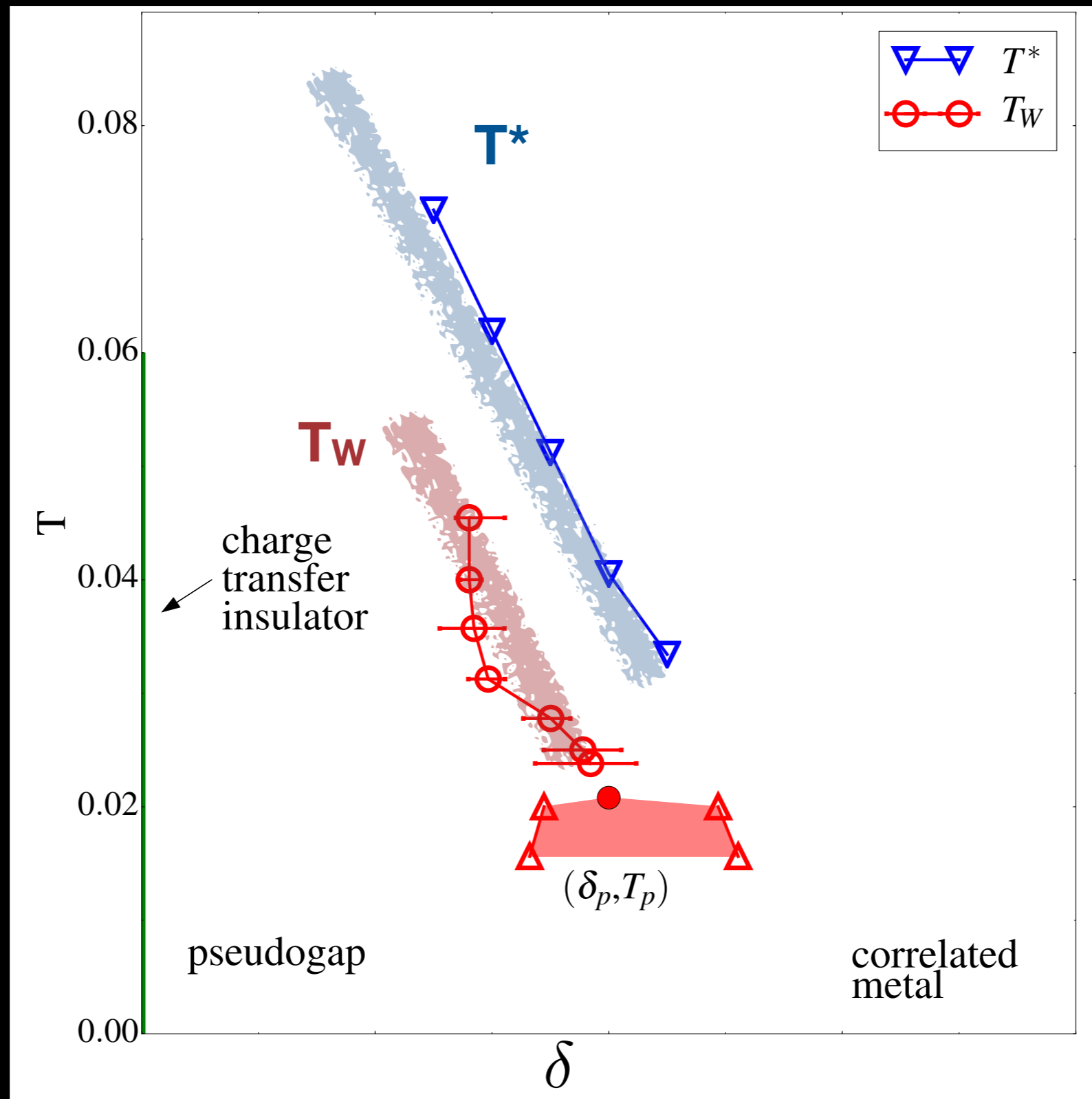
## Widom line:

continuation of the coexistence line in the supercritical region  
 line where the maxima of different response functions touch each other  
 asymptotically as  $T \rightarrow T_p$

# $T^*$ : onset of the pseudogap



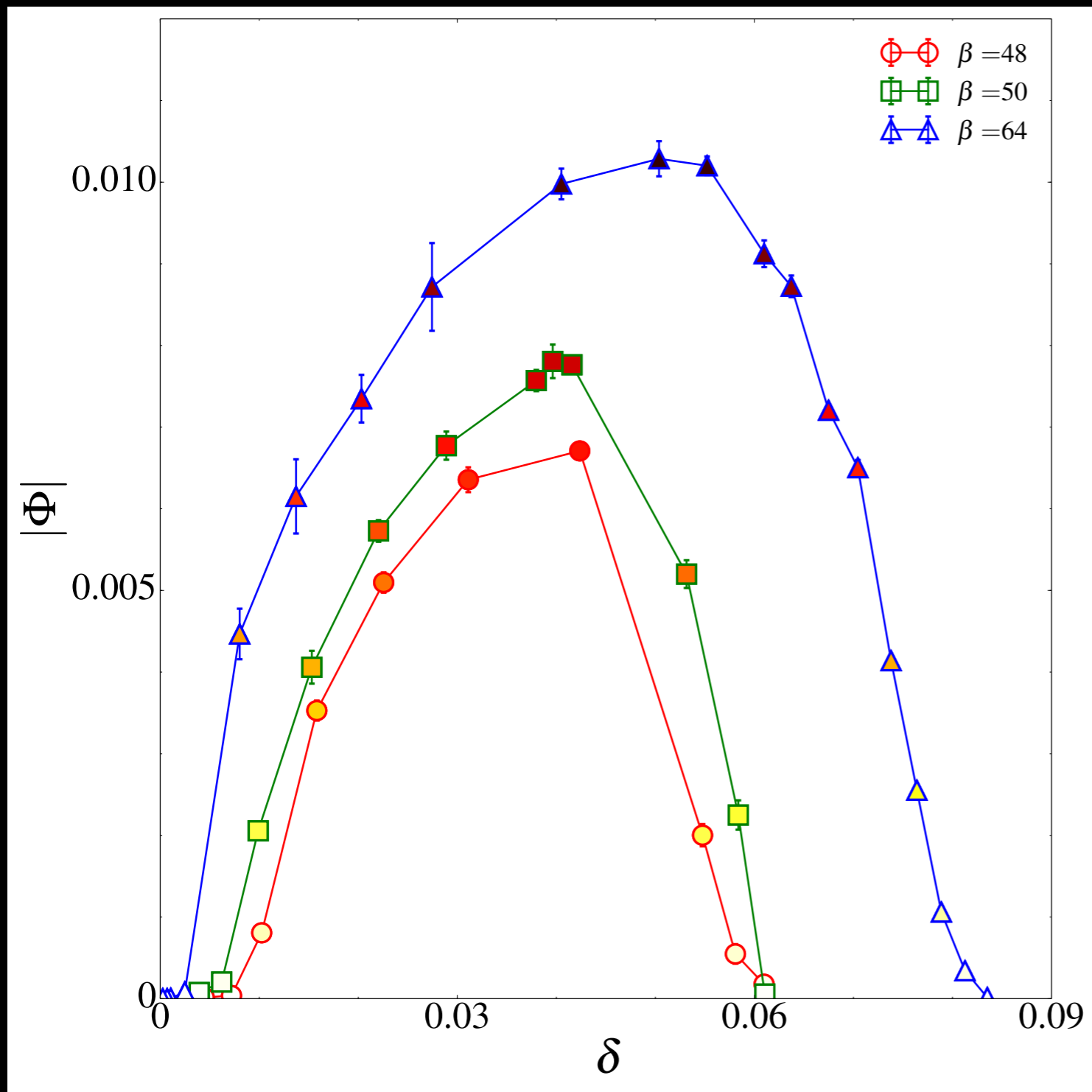
# hole-doping driven metal-insulator transition



$T_W$  :  
pseudogap  
temperature  
scale

$T^*$ :onset of  
the  
pseudogap  
(high  
temperature  
precursor of  
 $T_W$  )

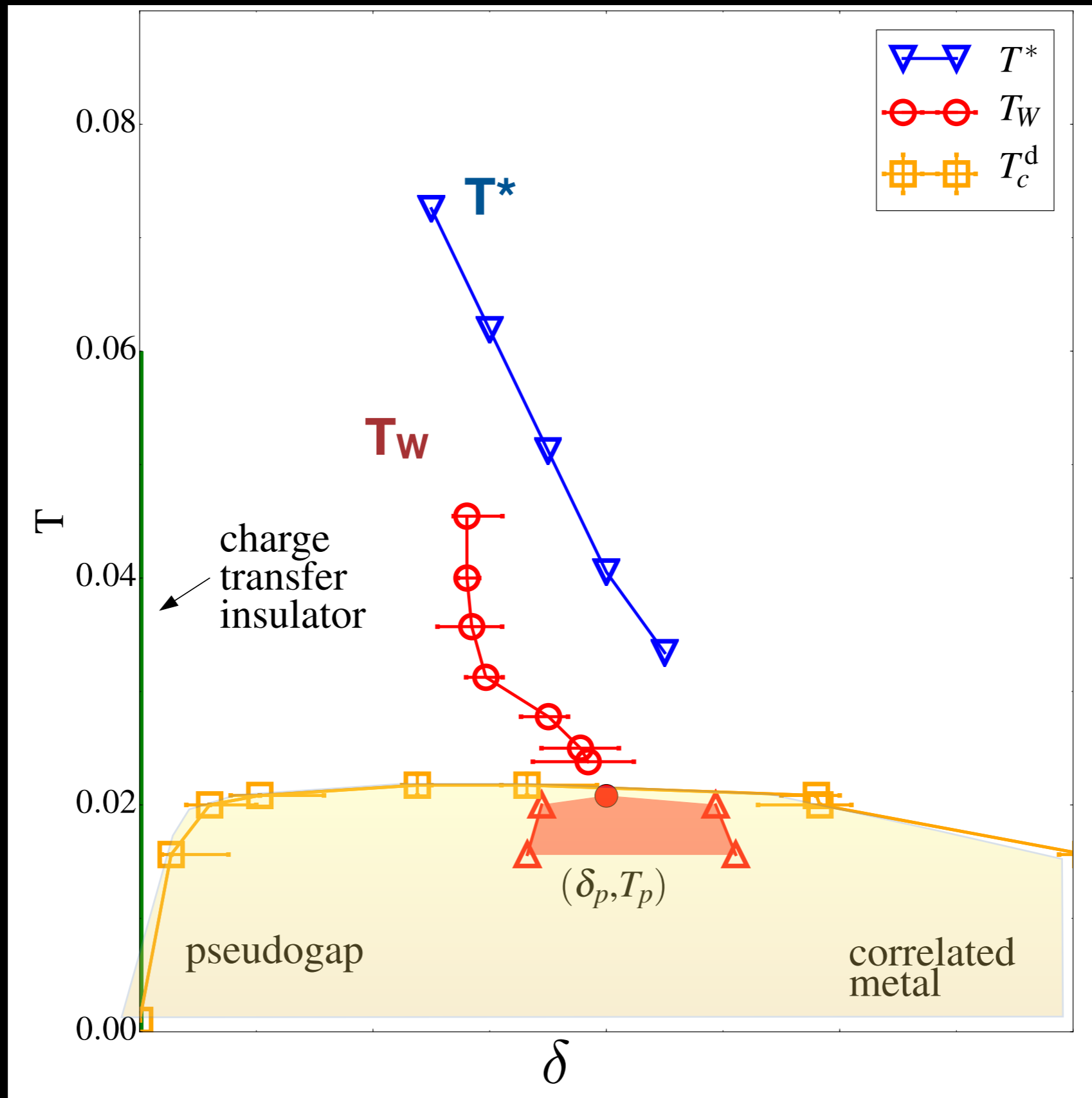
# Superconducting phase



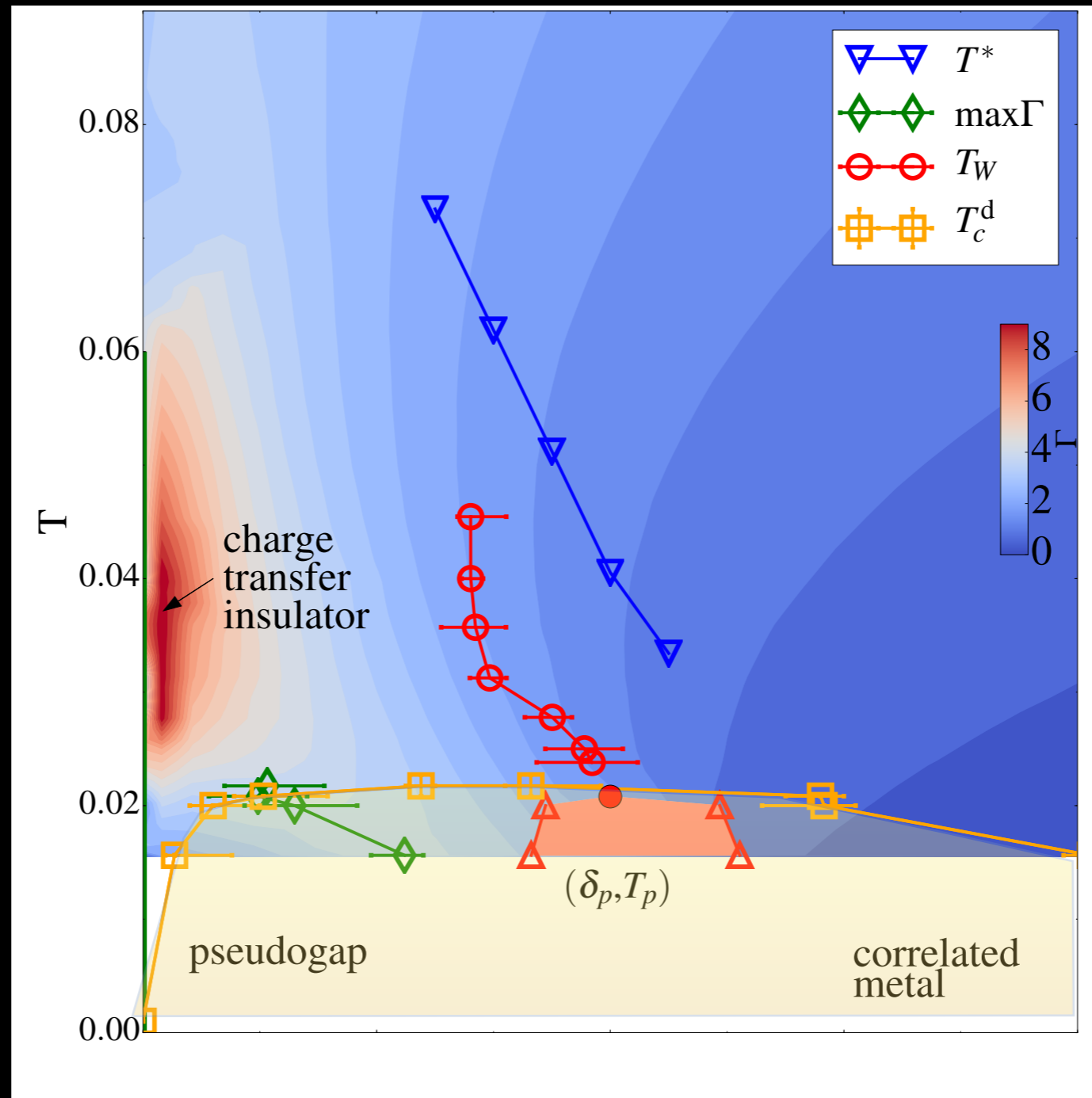
Order parameter:

$$|\Phi| \equiv |\langle \hat{d}_i^\dagger \hat{d}_j^\dagger \rangle|$$

# d-wave superconductivity

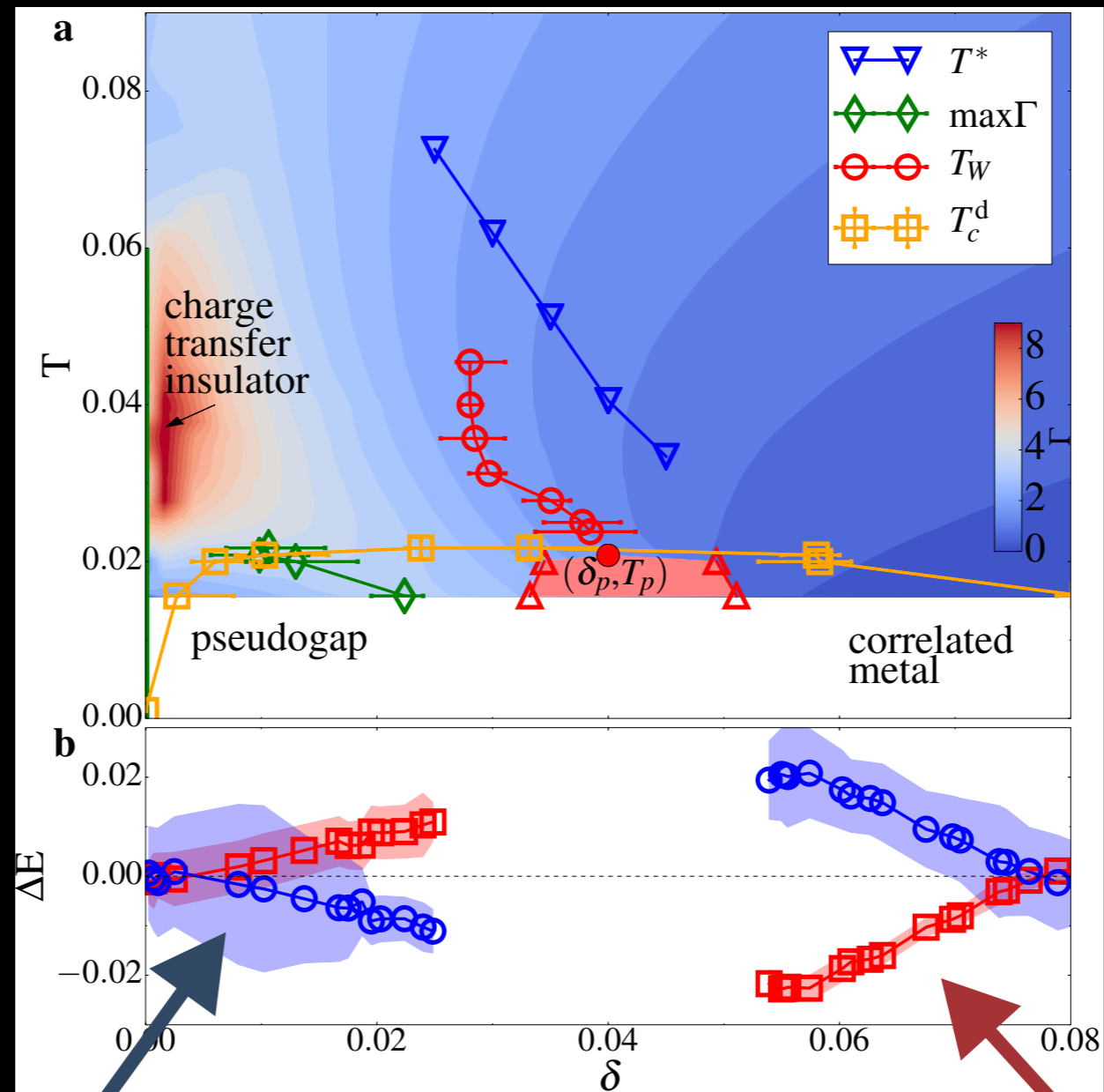


# d-wave superconductivity



**First order transition is the unifying feature of the self energy anisotropy**

# Condensation energy



kinetic energy driven SC

BLUE

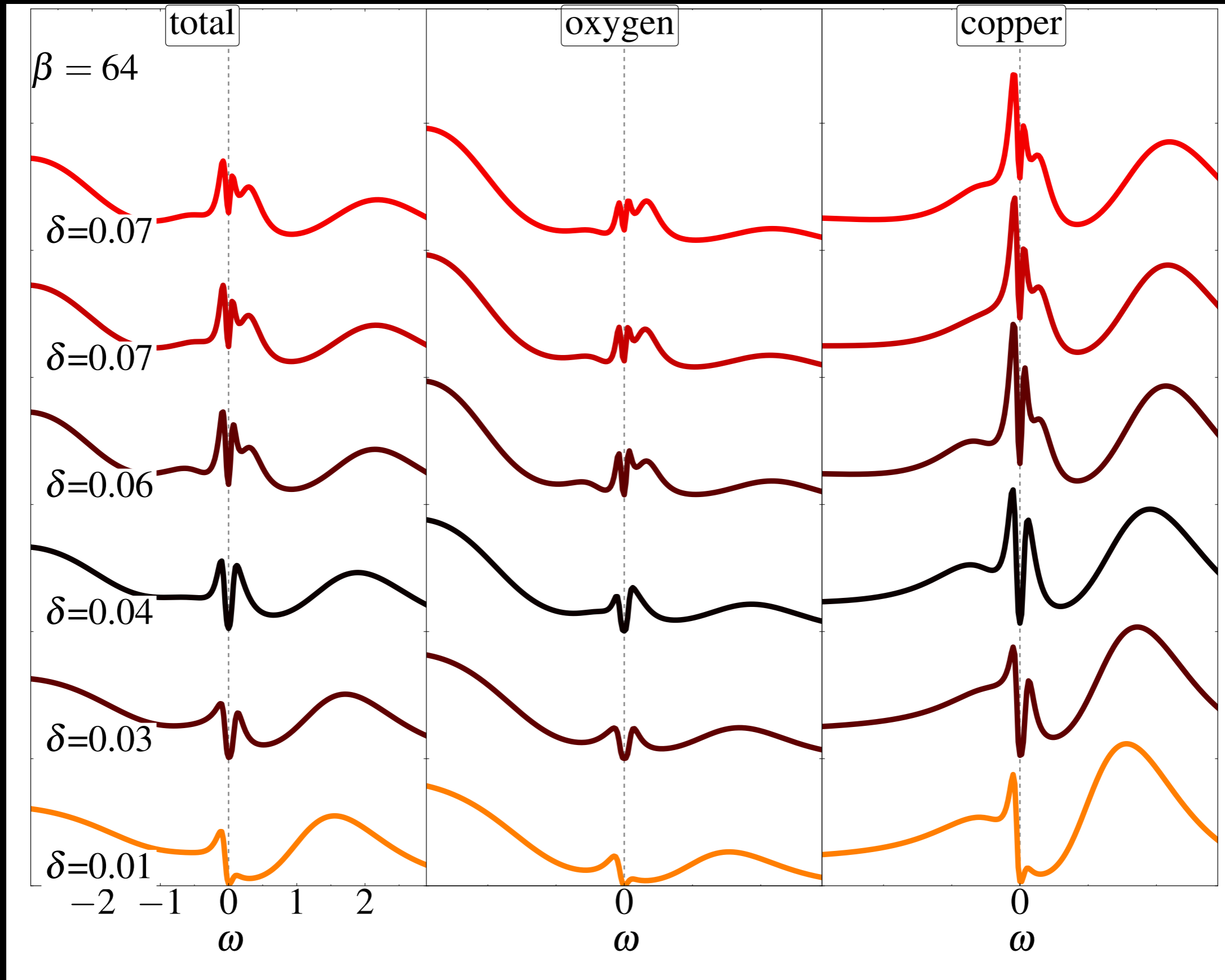
$$\Delta E_{kin} = E_{kin}^{SC} - E_{kin}^{NS}$$

RED

$$\Delta E_{pot} = E_{pot}^{SC} - E_{pot}^{NS}$$

potential energy driven SC

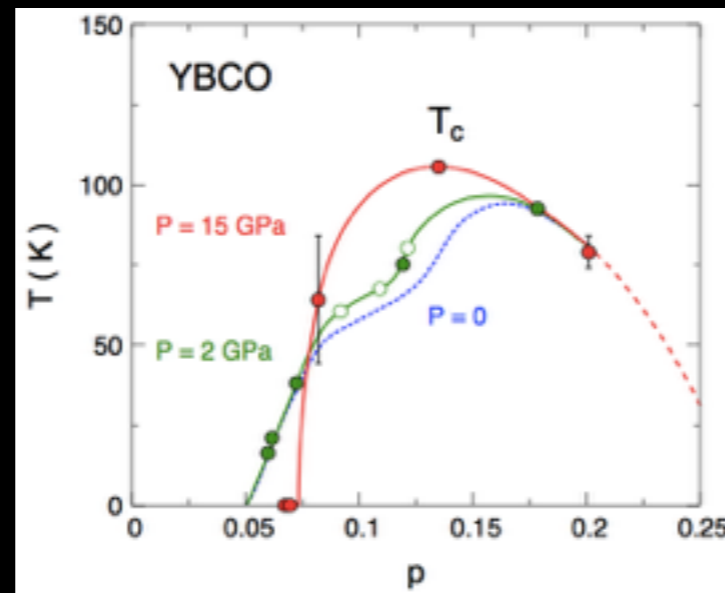
# d-wave superconductivity





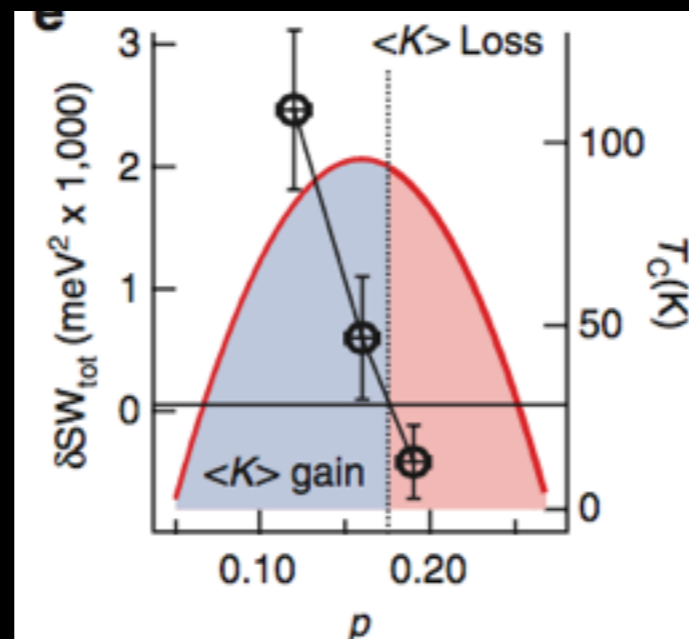
# d-wave superconductivity

1. why is there a dome and why is it shaped this way?



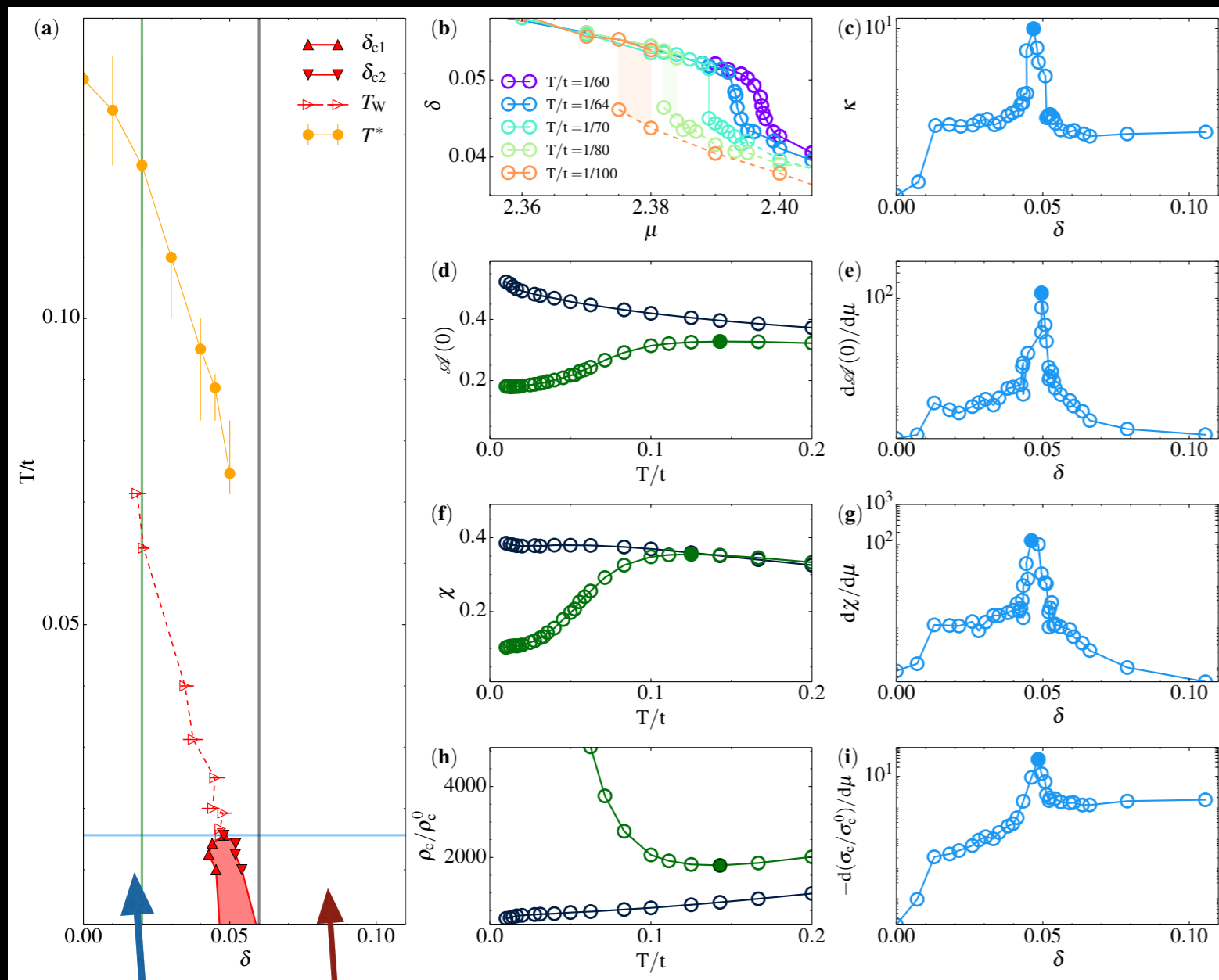
**Cyr-Choiniere et al,  
arXiv 2015;  
Sadewasser et al, PRB  
2000**

2. what drives the change from potential energy driven to kinetic energy driven SC?



**Giannetti et al, Nat Comm 2014;  
Deutscher et al, PRB 2005;  
Molegraaf et al, Science 2002;  
Carbone et al, PRB 2006**

# 1-band scenario: The first order transition as organising principle of the normal state



Above it a crossover line can be defined from characteristic anomalies of:

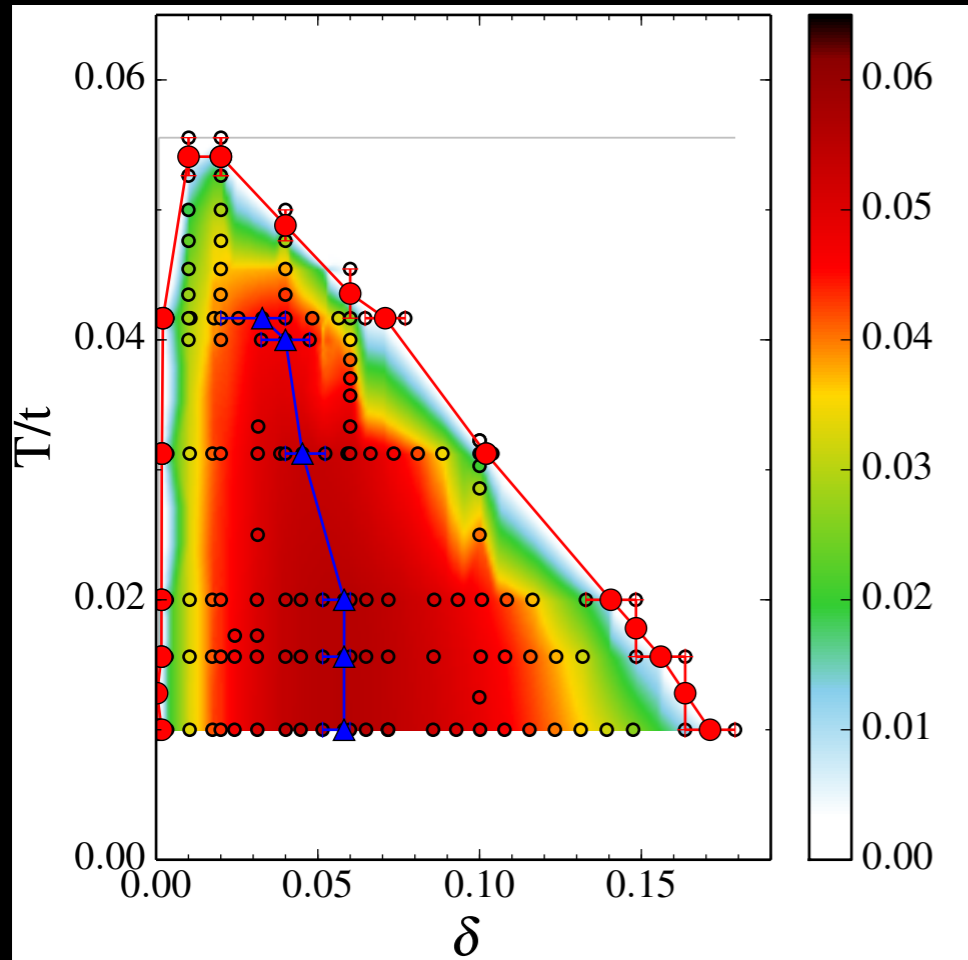
- thermodynamic
- dynamic
- transport

Correlated metal

Pseudo gap

Sordi G. et al., PRL (2010), PRB (2011), Sci. Rep. (2012)

# Superconducting state



Order parameter:

$$\Phi \equiv \langle \hat{c}_{\mathbf{K},\uparrow} \hat{c}_{-\mathbf{K},\downarrow} \rangle$$

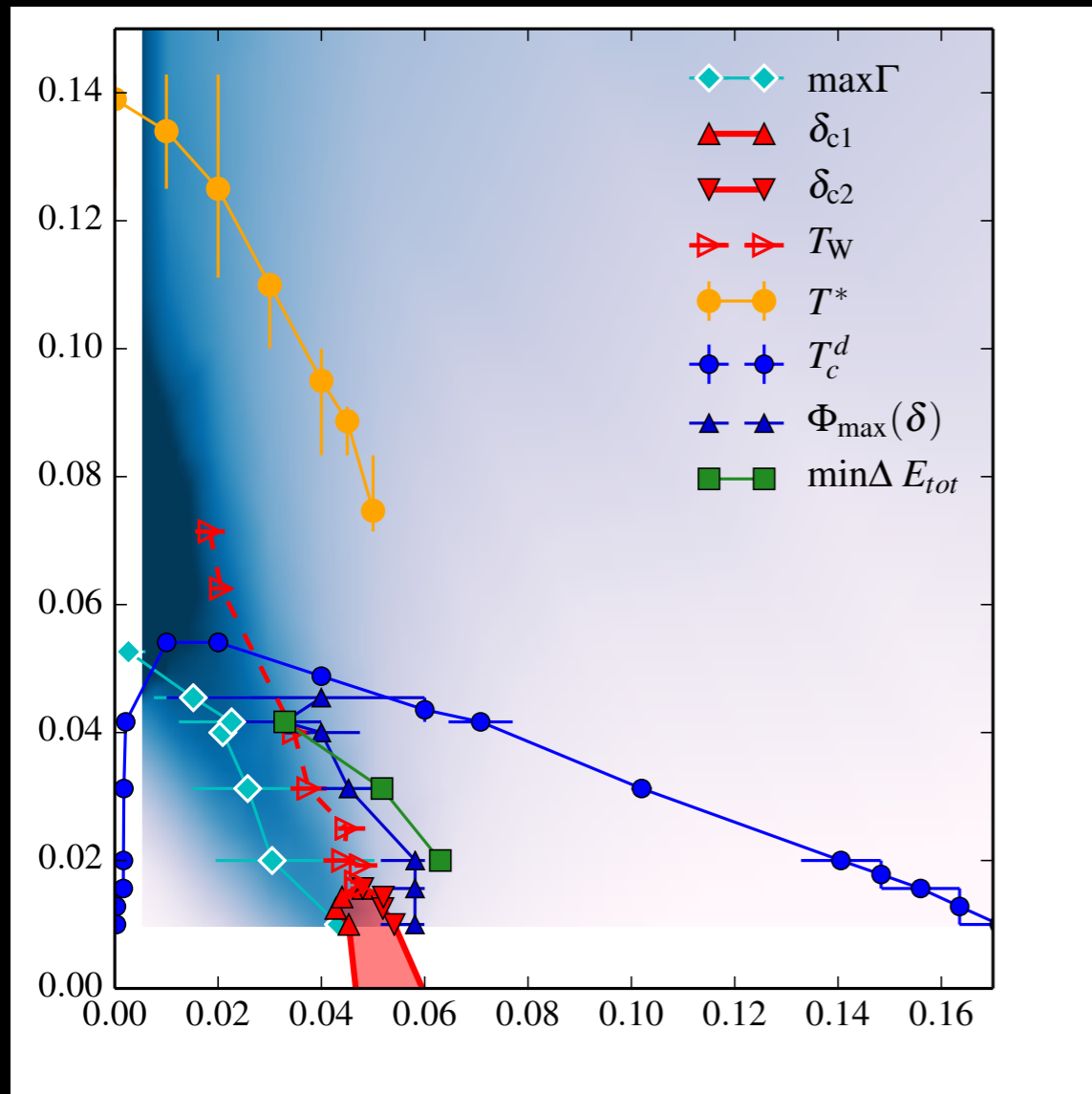
with  $\mathbf{K} = (\pi, 0)$

**Tc does not scale with  $\phi$**

**asymmetry of SC dome is linked to  $\phi_{\max}$**

**L. Fratino et al., Scientific Reports 6, 22715 (2016)**

# The organising principle of SC

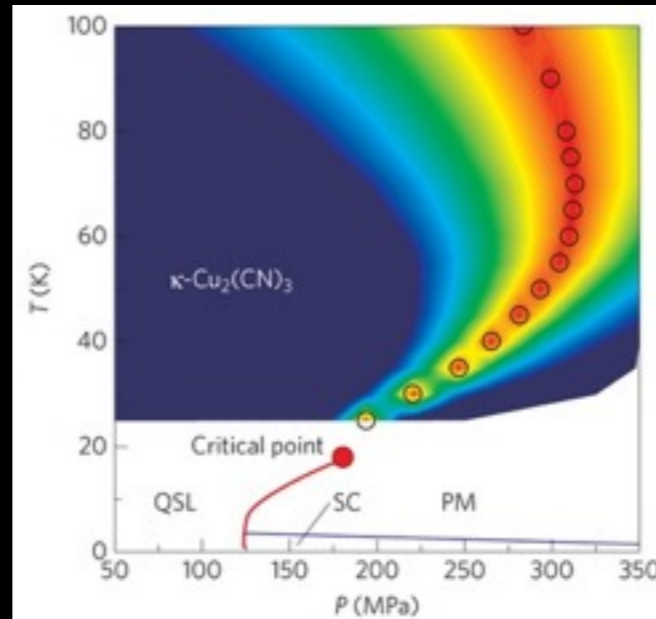


- $\phi_{\max}$  closely parallels to  $T_W$
- $\phi_{\max}$  closely parallels to  $\Gamma_{\max}$
- $\Gamma_{\max}$  crosses  $T_c$  at  $\delta_{opt}$
- SC emerges from pseudo gap or from correlated metal
- condensation energy parallels  $\phi_{\max}$

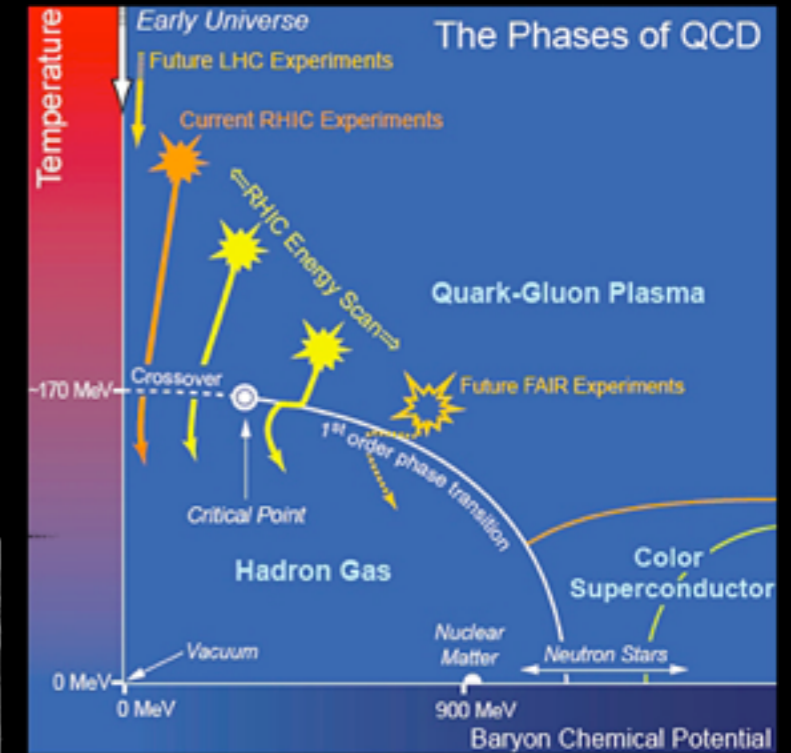
**superconductivity and pseudogap are intertwined phenomena**

Widom line found in k-organics!

**Furukawa, Nat. Phys. (2015)**

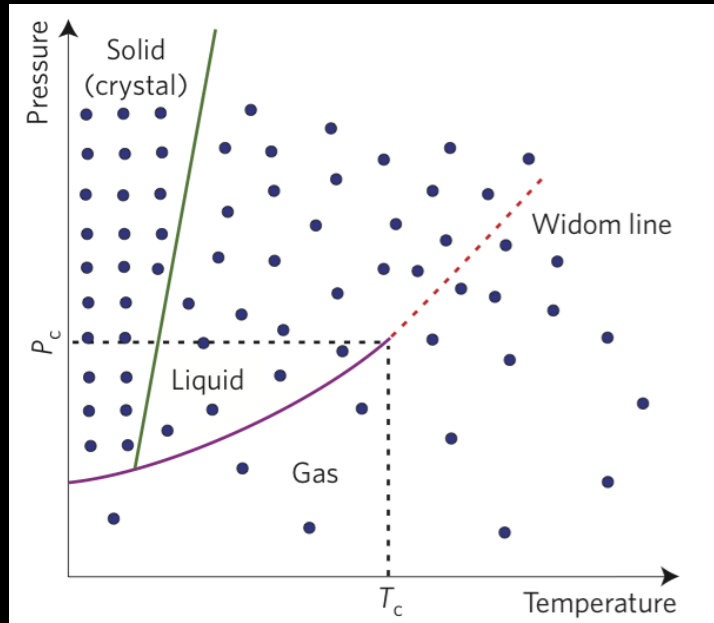


Widom line in the QCD phase diagram?

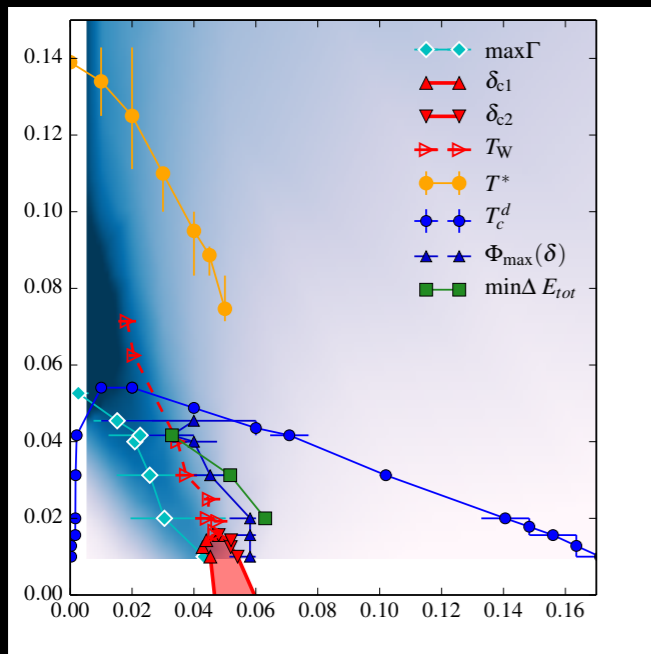


Widom line found in water

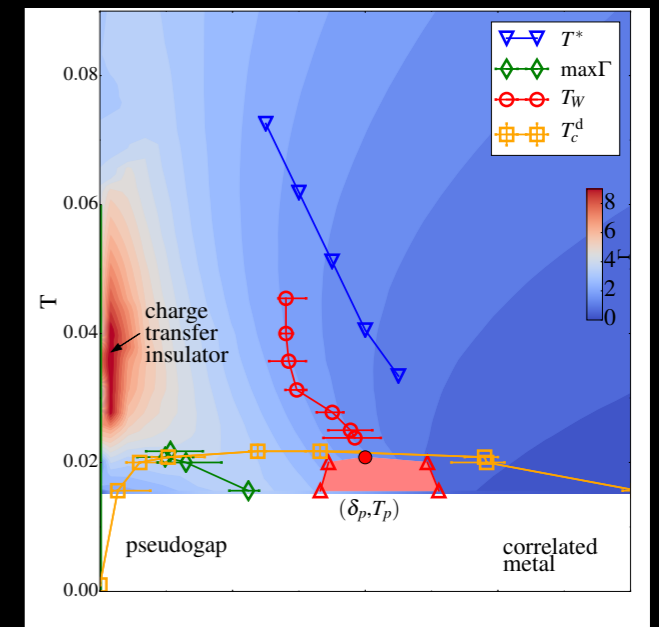
**McMillan and Stanley, Nat Phys 2010**



**Widom line a universal organising principle in physics!**



**L. Fratino et al., Scientific Reports 6, 22715 (2016)**



**L. Fratino et al., Phys. Rev. B 93, 245147 (2016)**

**I am currently looking for a postdoc**



**Do you have funding for the next year?  
Let's talk about it!**

**Thank you for the attention!**