# Basic model for high-$T_c$ cuprates

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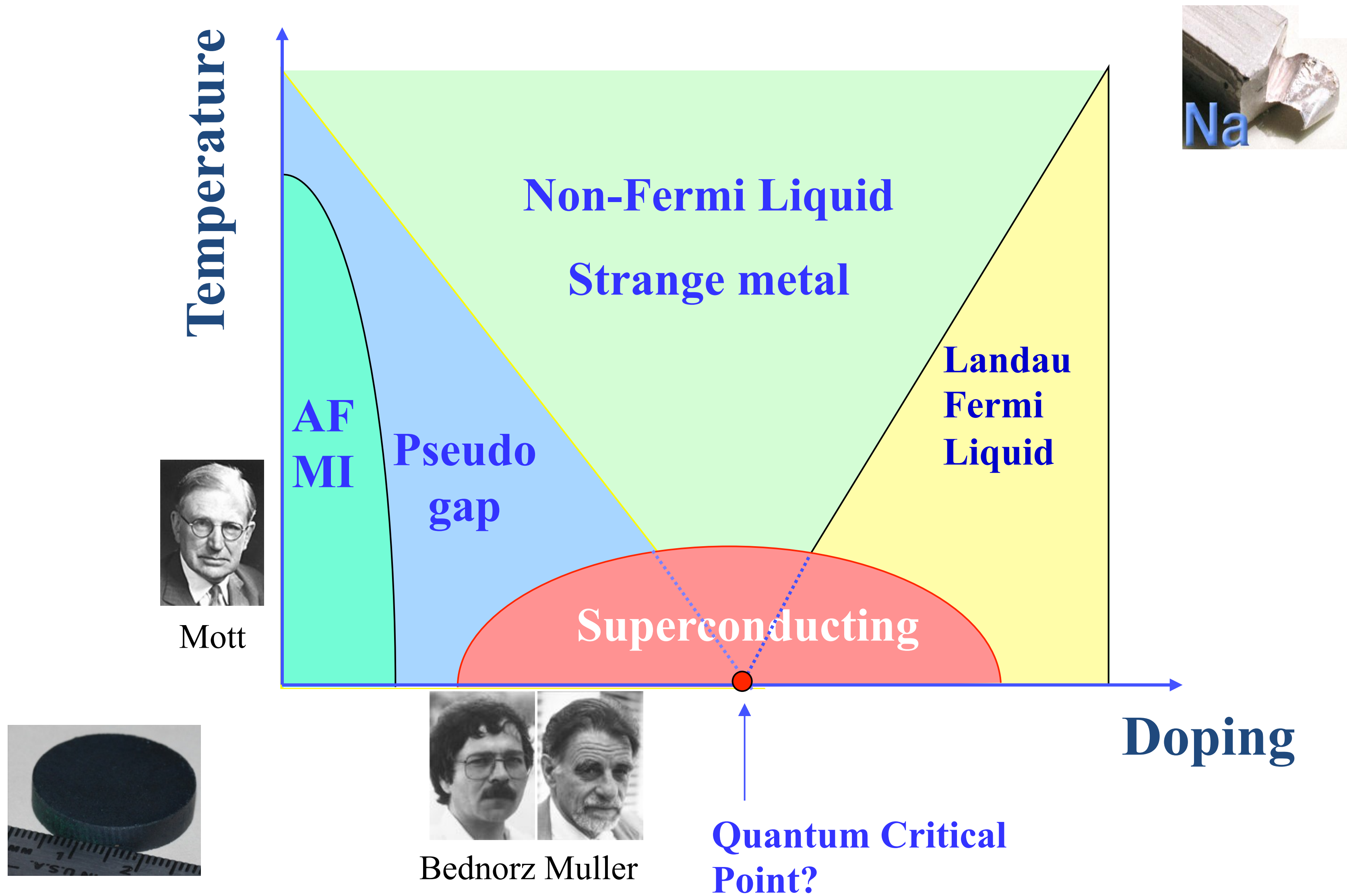
# outline

- Brief introduction and basic model for hole-doped cuprates

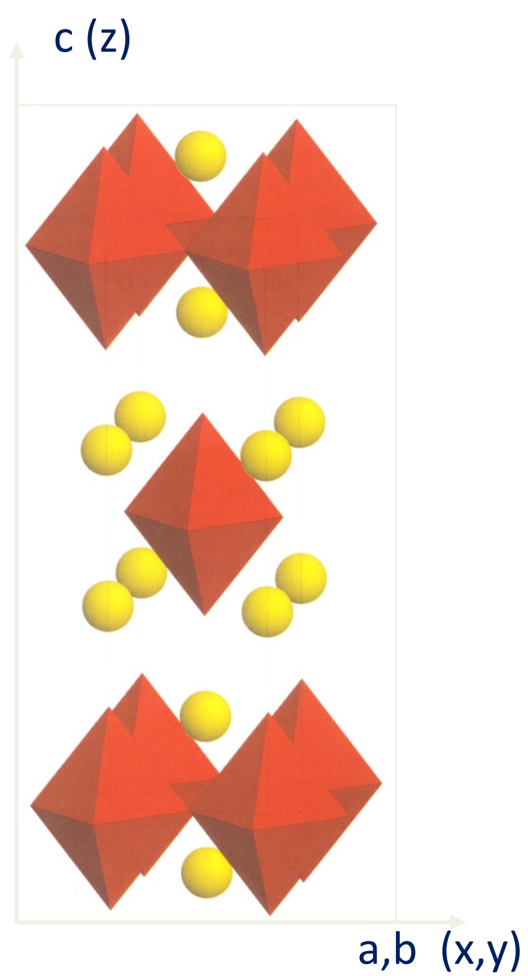
- basic model for Electron-doped

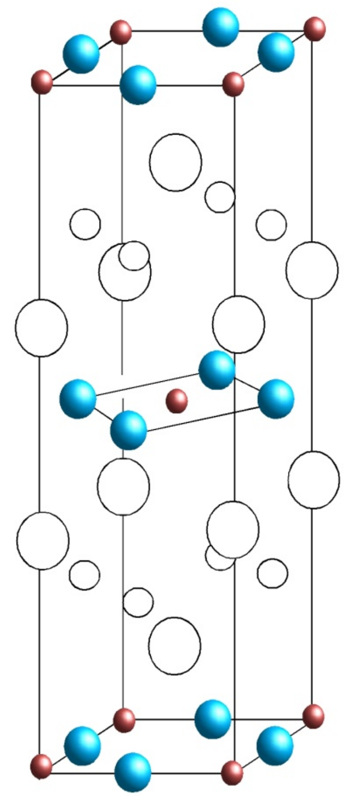
- Electronic structure along the c-axis

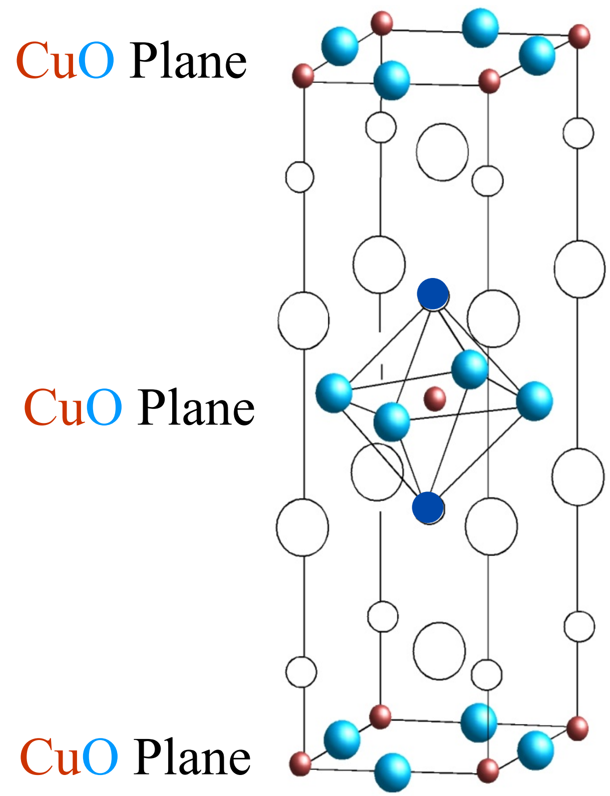
# Phase Diagram: High-Tc Cuprates



# Crystal Structure






n-doped

$(Nd,Pr,Sm)_{2-x}Ce_xCuO_4$

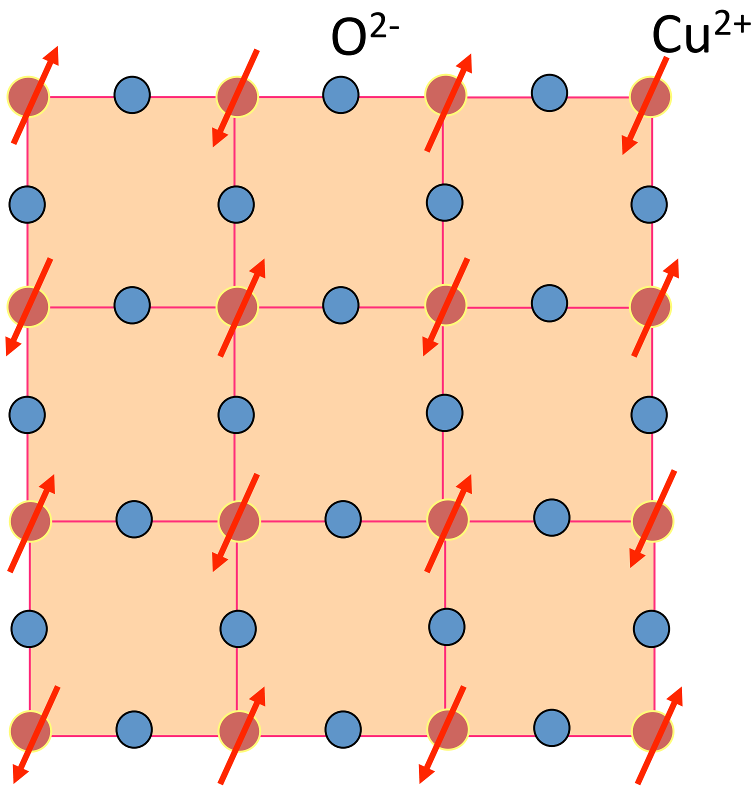
electron doped

p-doped

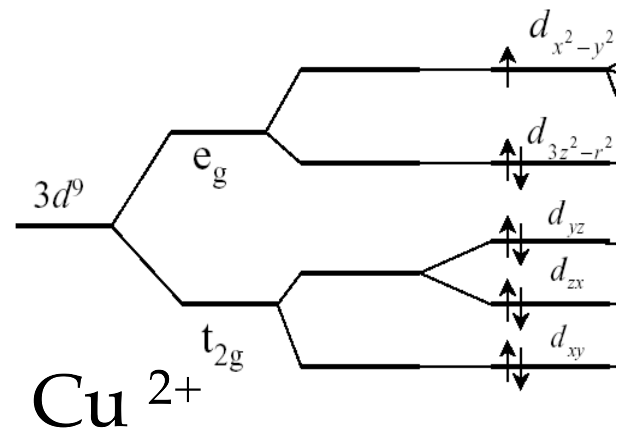
$La_{2-x}Sr_xCuO_4$ $(HgBa_2CuO_{8+\delta})$

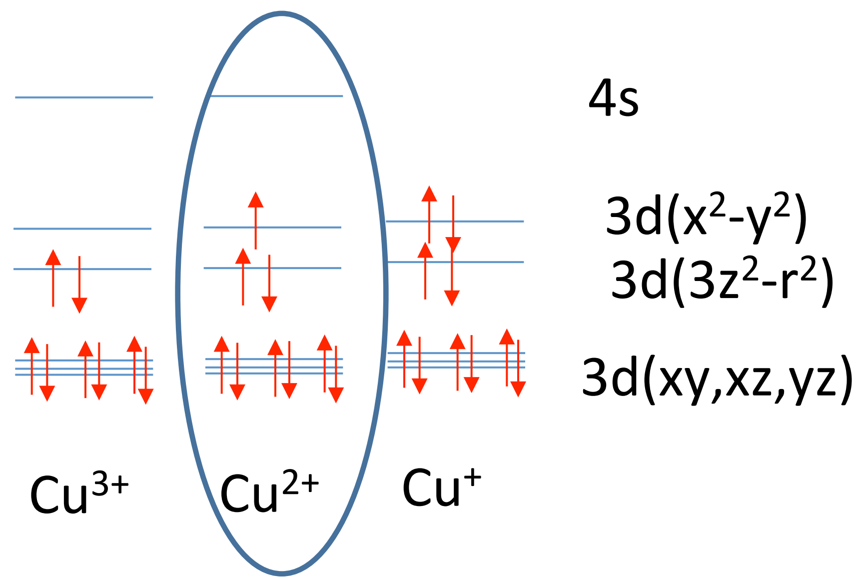
hole doped

# Undoped CuO plane

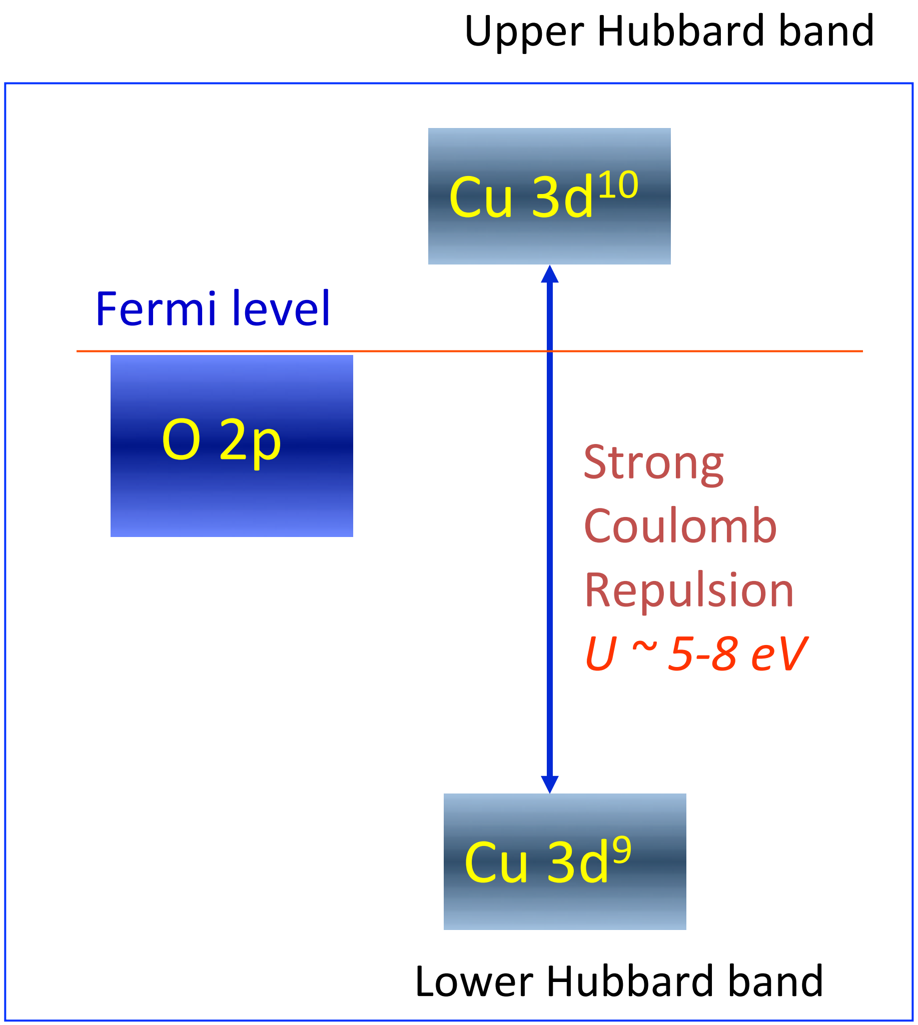


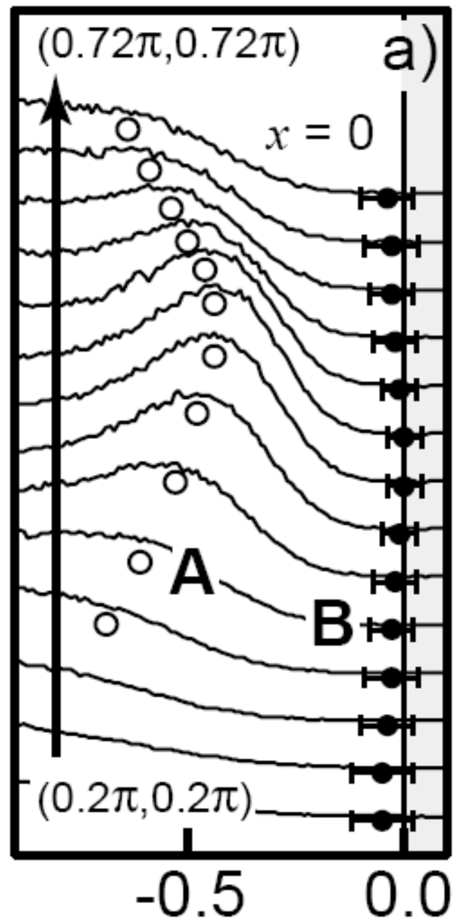

$T_N$ ~ 500K



# Undoped CuO plane



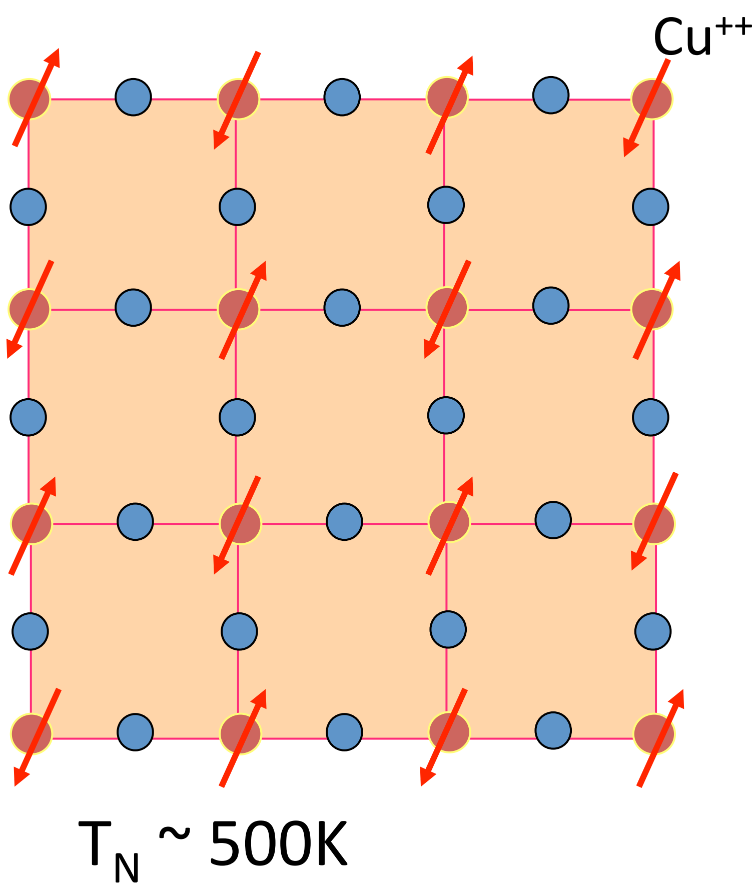

$Ca_2CuO_2Cl_2$

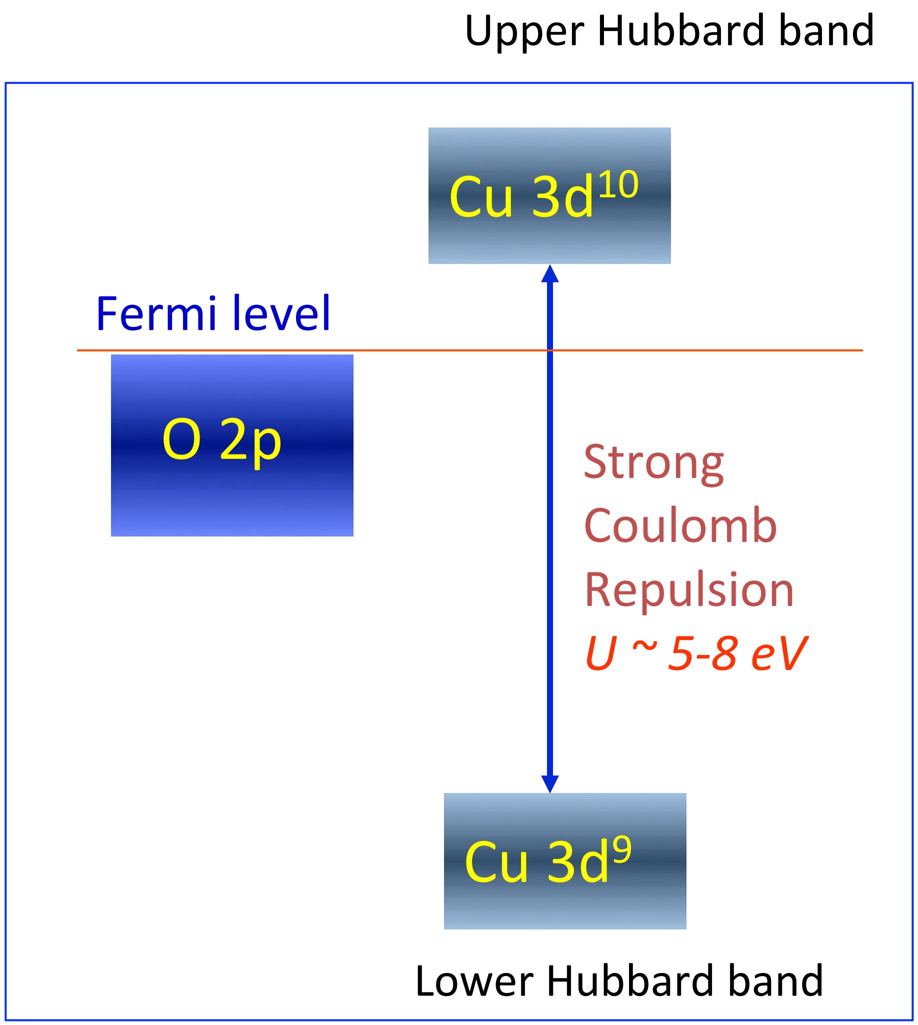
Shen et al, PRL 2004

# Parents: Antiferromagnetic Mott insulator

Heisenberg

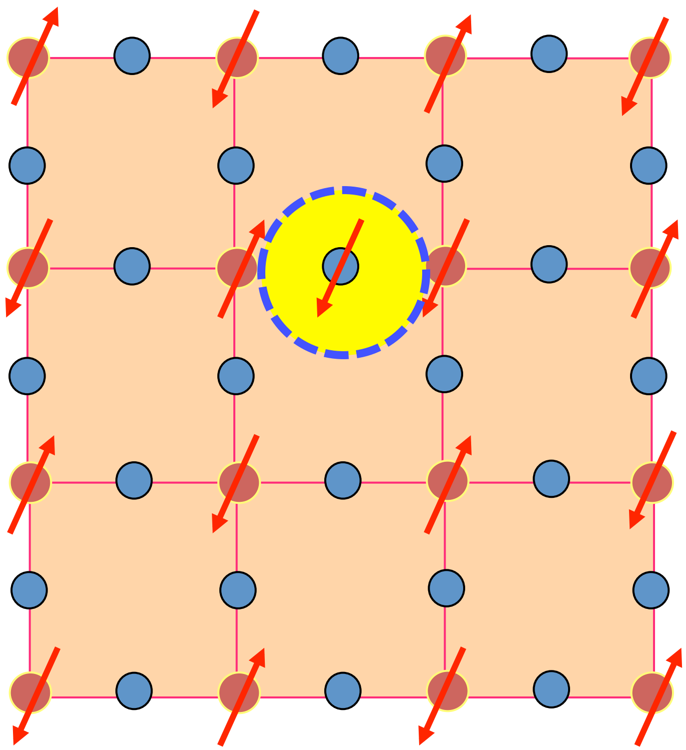
$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j$$



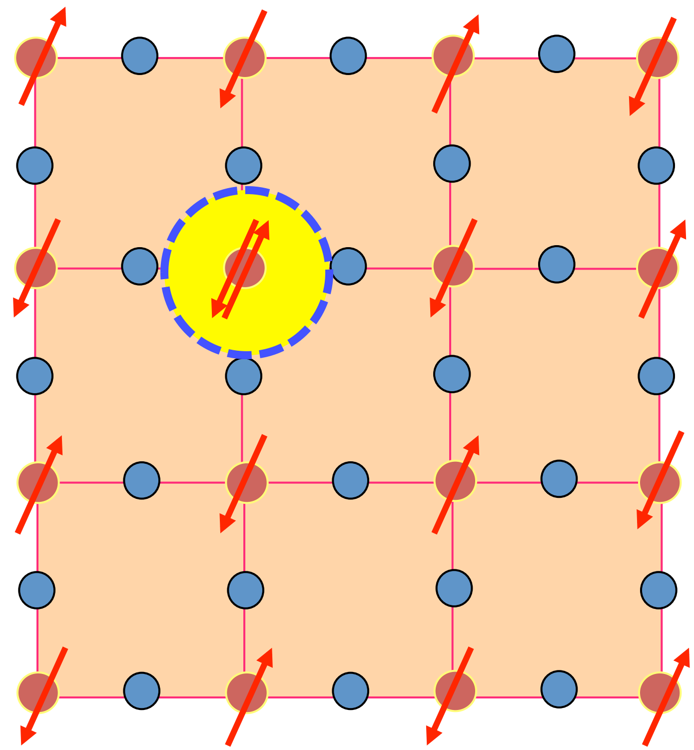



# Doped cuprates

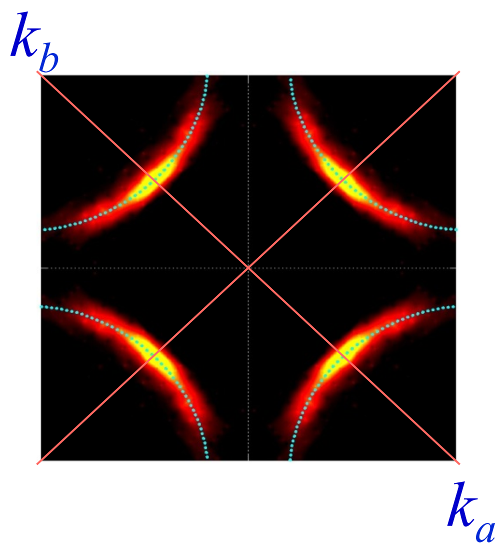
Hole doping: on O site

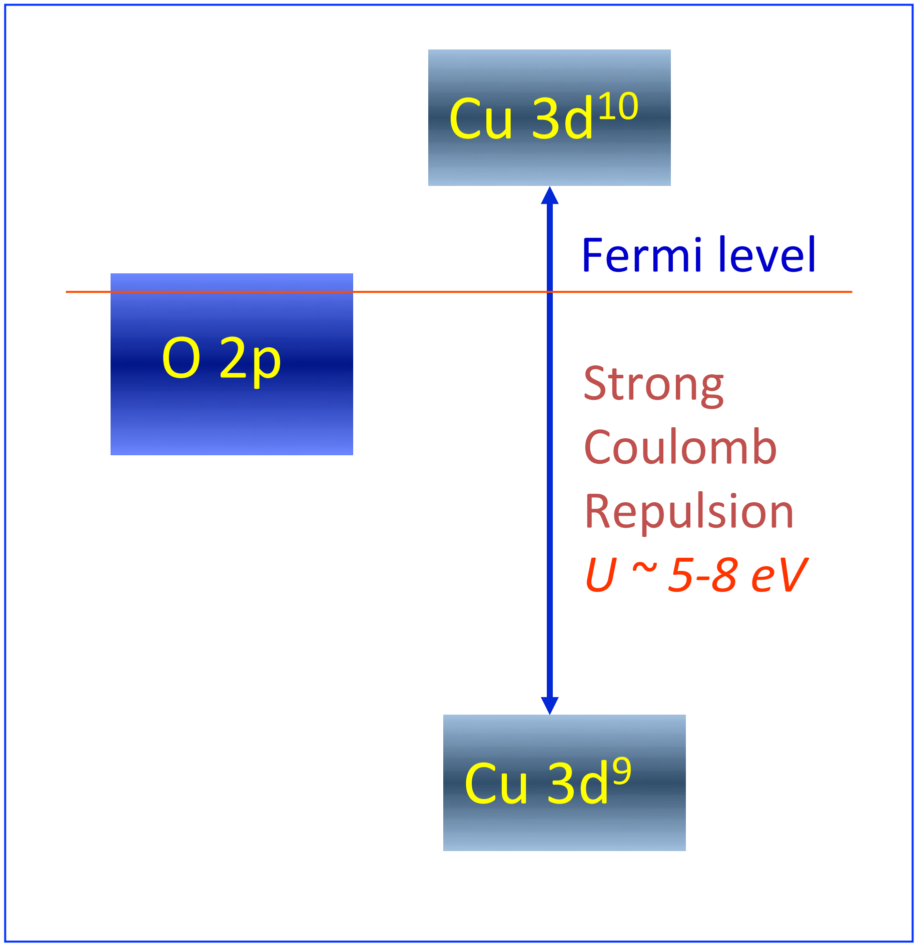


Electron doping: on Cu site

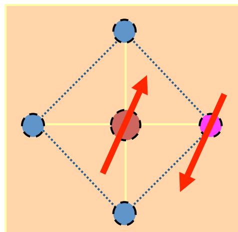


# Hole doping

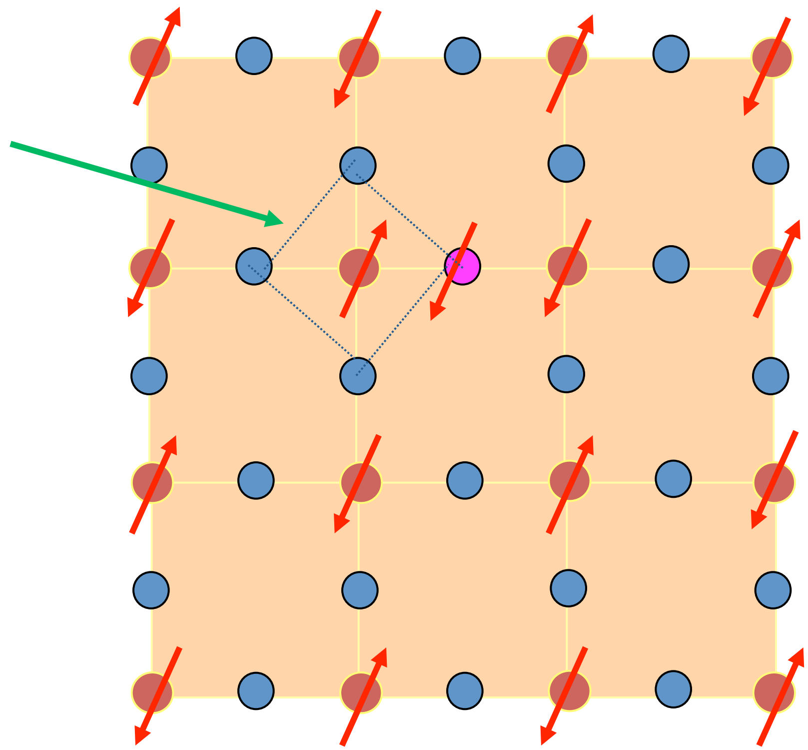

$k_b$
$k_a$


Cu 3d$^{10}$
Fermi level
O 2p
Strong
Coulomb
Repulsion
$U$ ~ 5-8 eV
Cu 3d$^{9}$

# Hole doped cuprates: t-J model



**Zhang-Rice Singlet**



**Band width**

**tight binding ~ 8t**

**t-J model ~ 2J**

FC Zhang TM Rice

Zhang-Rice singlet

$$H = -t \sum_{\langle ij \rangle} c_i^+ c_j + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$c_i^+ c_i \leq 1$$

Kinetic energy spin-spin interaction

# Slave boson representation of the t-J model

Spinon holon

$$\mathcal{H} = -t \sum_{\langle ij \rangle} d_i^+ h_i d_j h_j^+ + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$c_{i\sigma}^+ = d_{i\sigma}^+ h_i$$

$$d_i^+ d_i + h_i^+ h_i = 1$$

$$H = -t \sum_{\langle ij \rangle} c_i^+ c_j + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$c_i^+ c_i \leq 1$$

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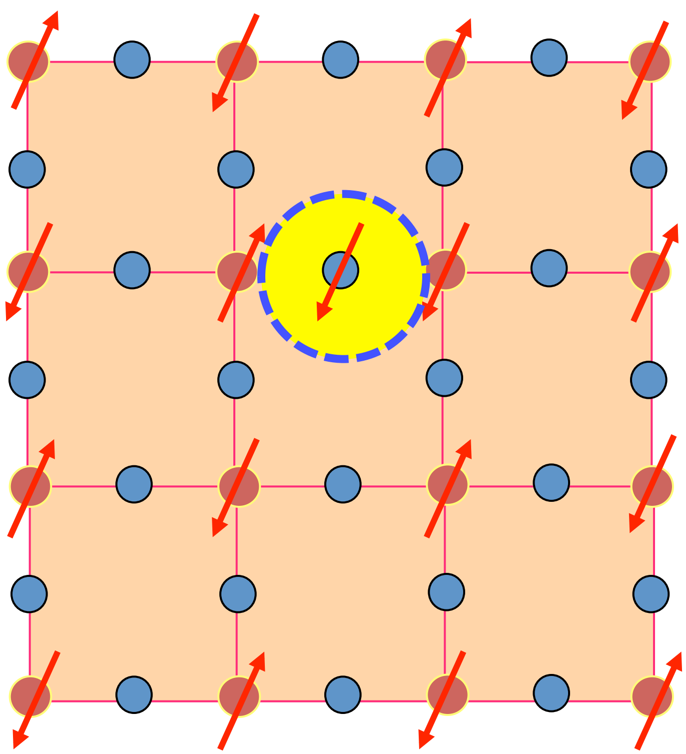
# Minimal Model

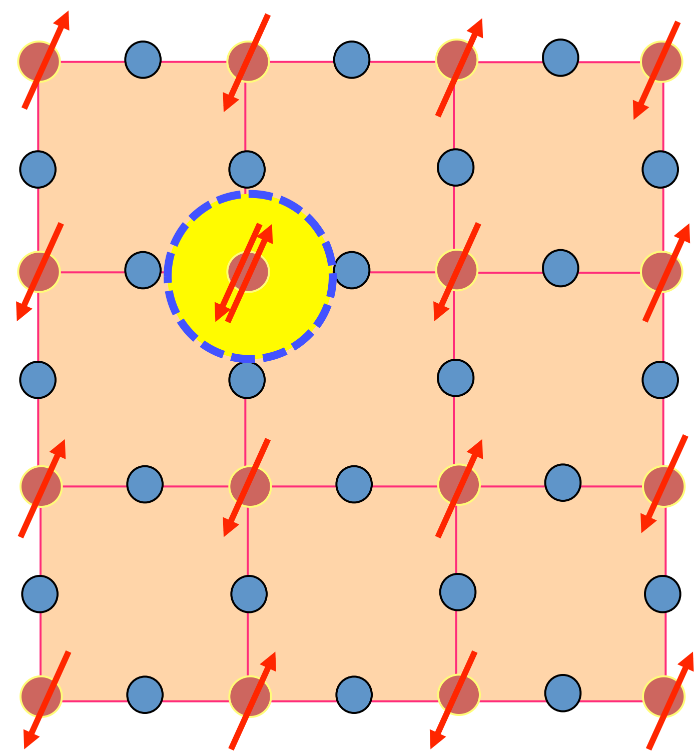
Hole doping: on O site

Electron doping: on Cu site

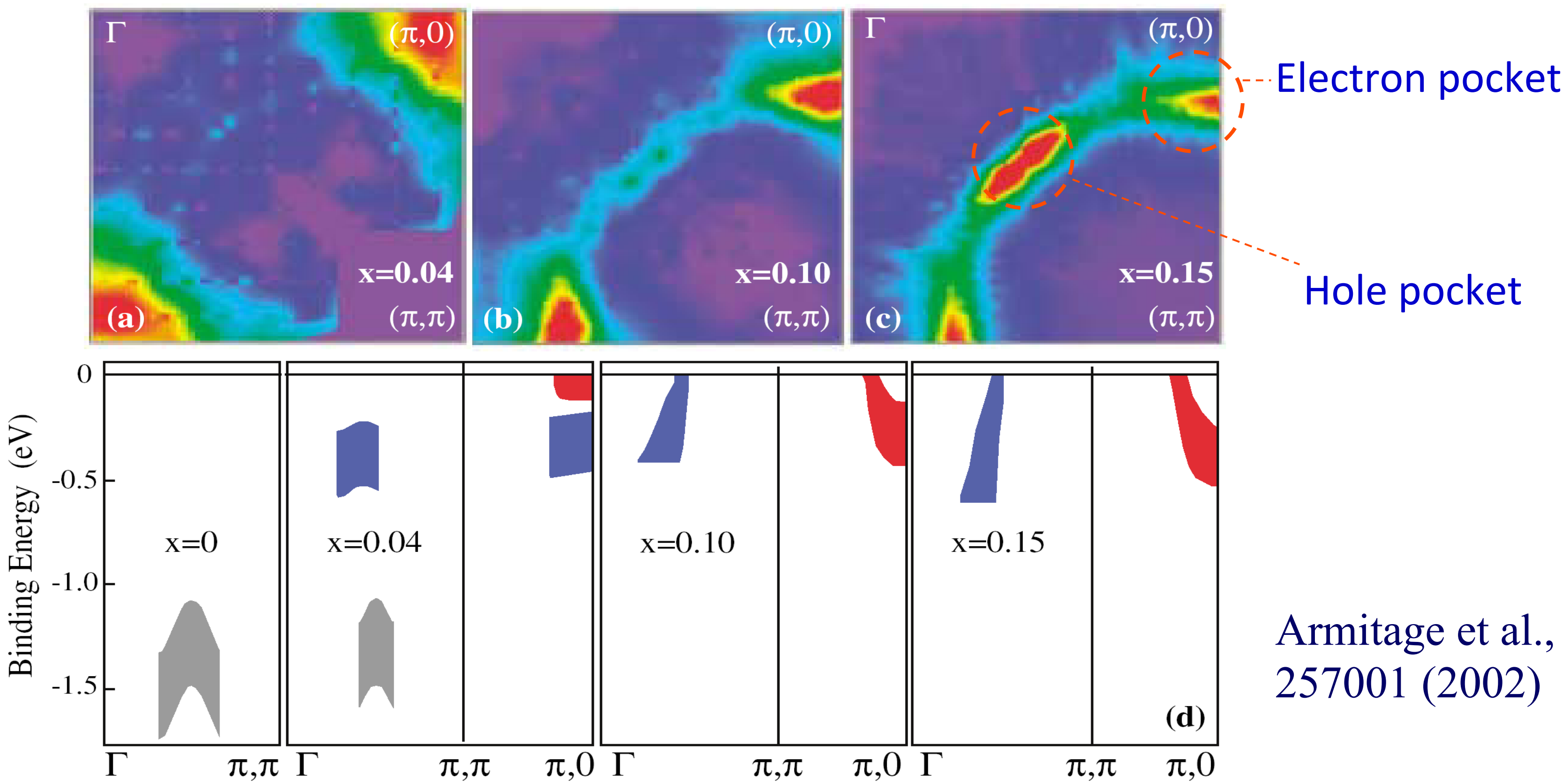
$$H = -t\sum_{<ij>}\left(\tilde{c}^{+}_{i\sigma}\tilde{c}_{j\sigma} + h.c.\right) + J\sum_{<ij>}\vec{S}_i \cdot \vec{S}_j$$

?





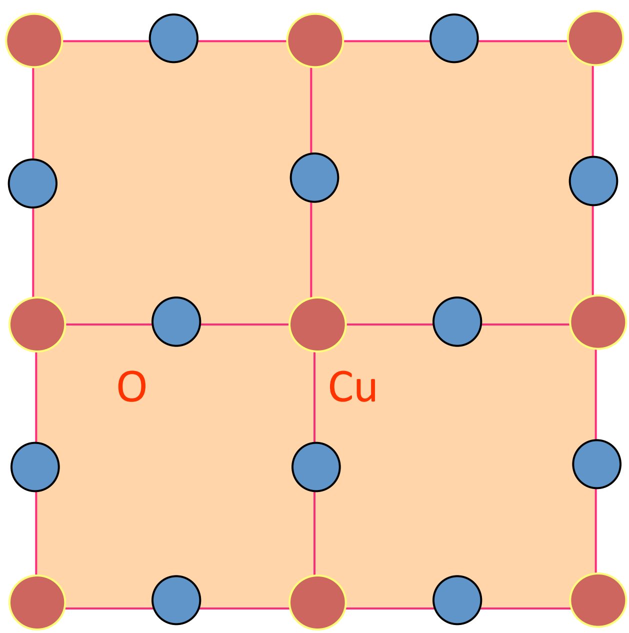
# ARPES: Doping evolution of the Fermi Surface

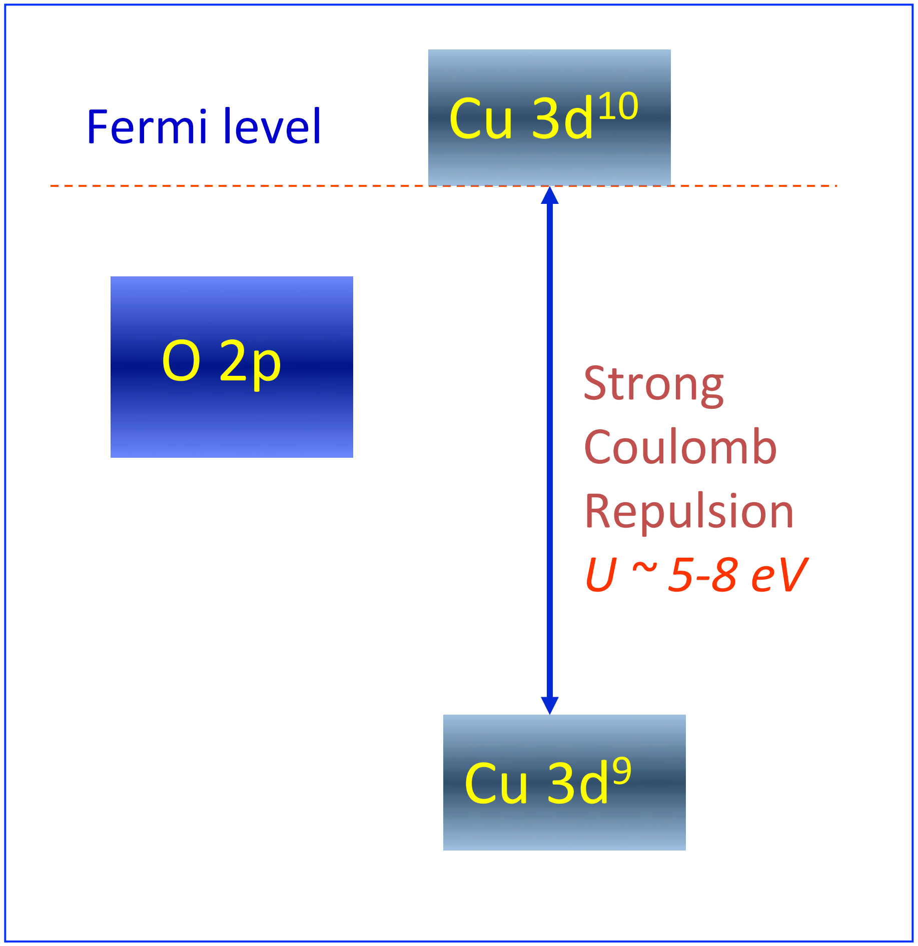



Armitage et al., PRL 88, 257001 (2002)

Increasing doping, Fermi surface first appears at (π,0)
then at (π/2, π/2)

# Where are the two bands from?



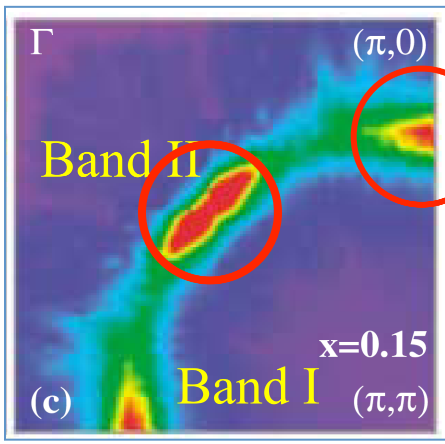




Luo, Xiang, PRL **94** (2005) 027001

# Origin of the two bands: underdoping overdoping

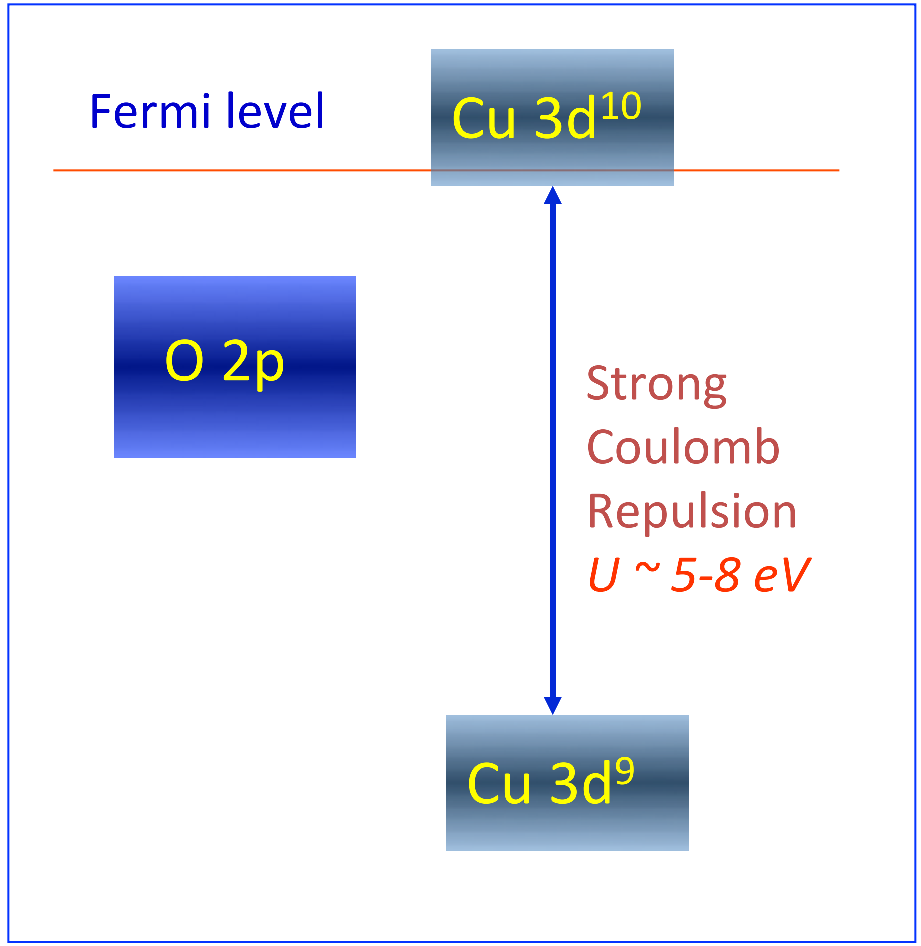
Electron pocket:

Cu $3d^{10}$ band

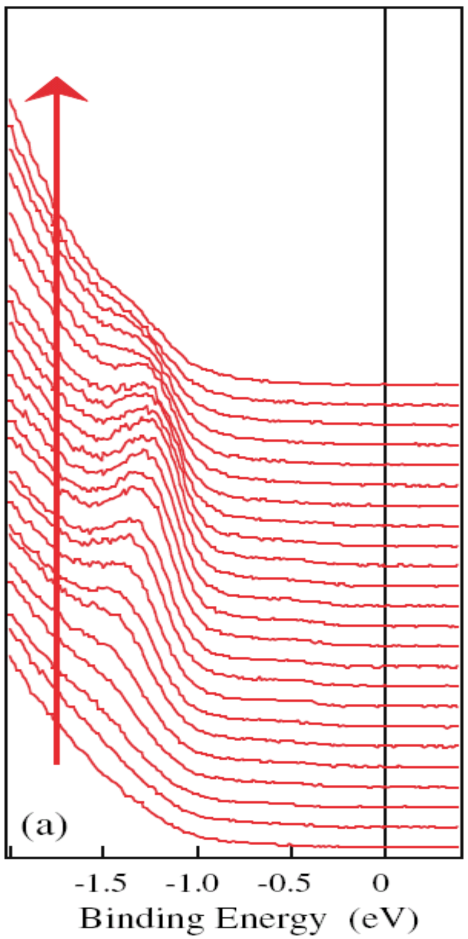



Hole pocket:

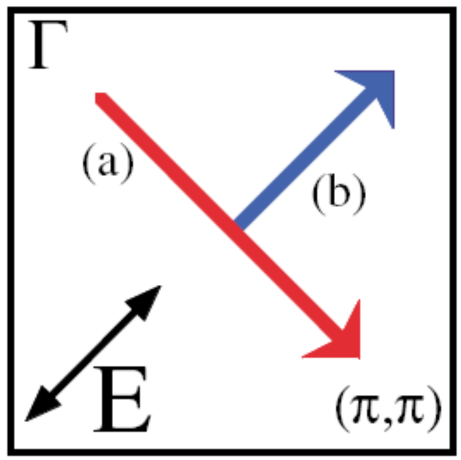
Zhang-Rice singlet band



# Doping evolution of electronic structure: Zero doping




There is a dispersive band about 1.2 eV below the Fermi level

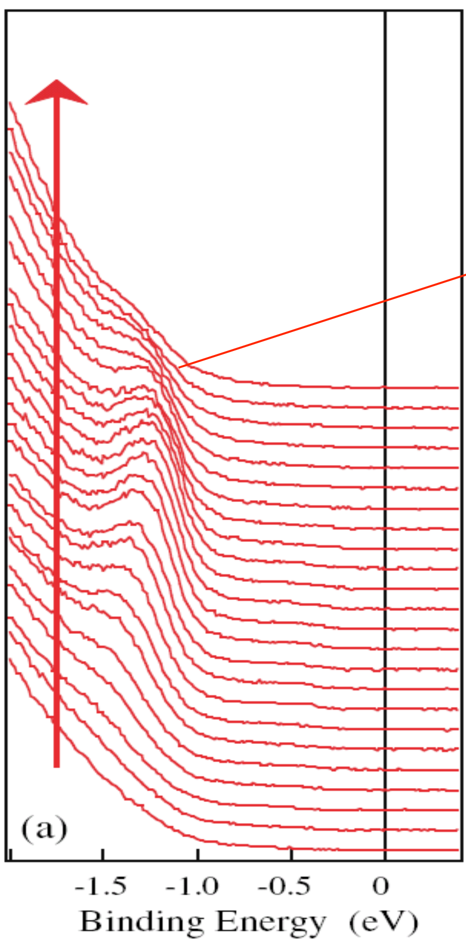



$Nd_2CuO_4$

Parent compound of electron doped materials

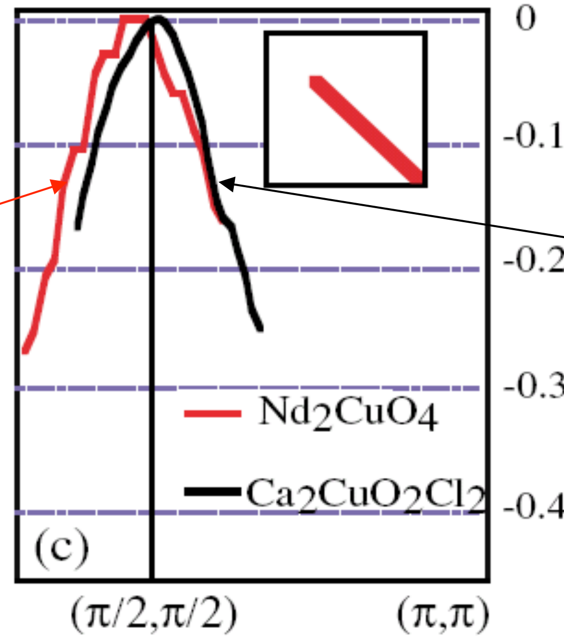
Armitage et al, PRL 2002

# Doping evolution of electronic structure: Zero doping

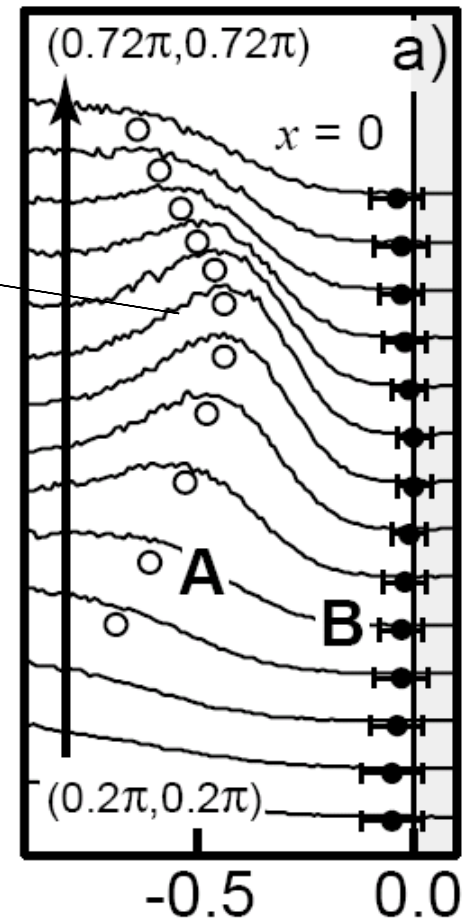



$Nd_2CuO_4$

Armitage et al, PRL 2002




Momentum dependence of the peak energy with respect to the minimal excitation gap



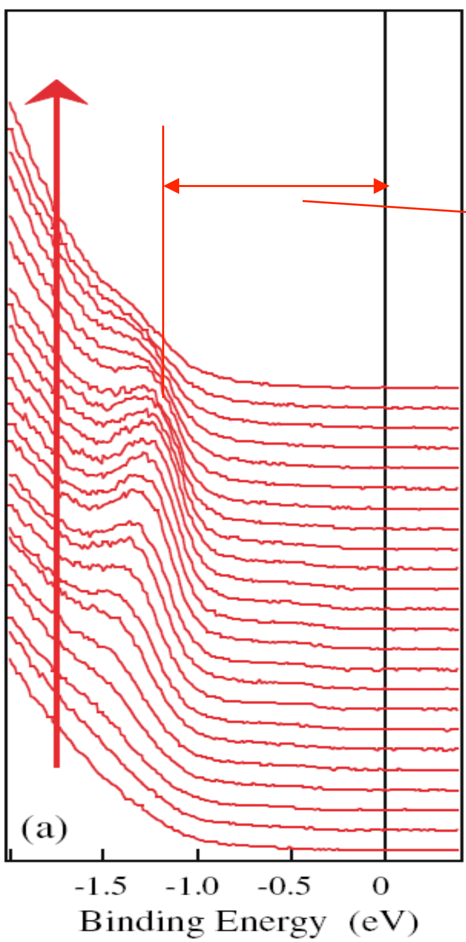

$Ca_2CuO_2Cl_2$

Shen et al, PRL 2004

# Where is the Fermi level?

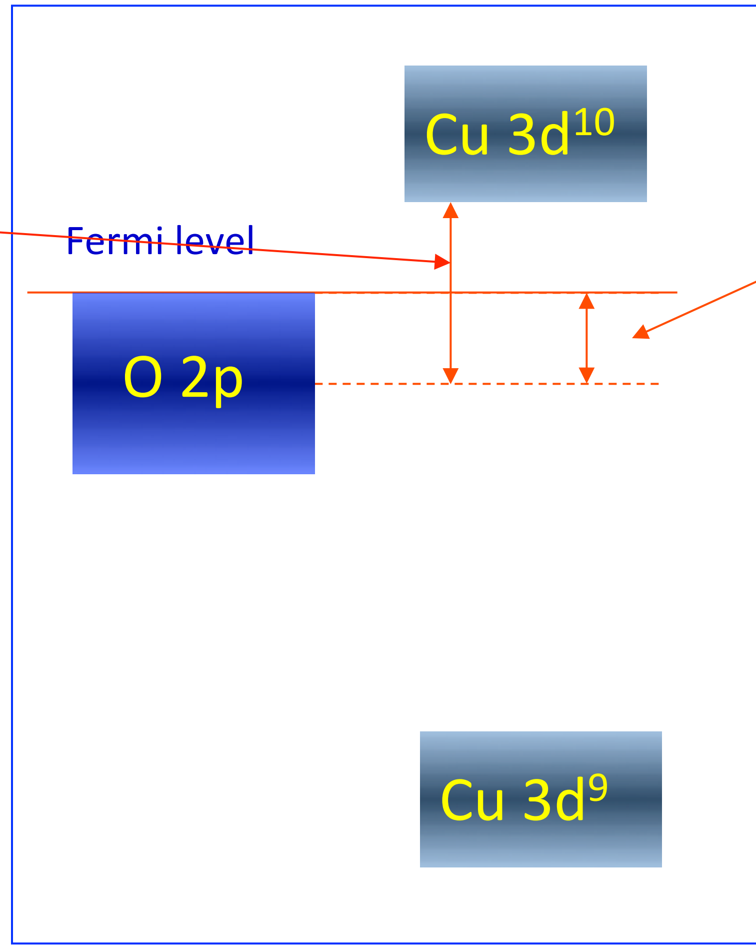
Fermi level pinned at bottom of UHB due to slight oxygen nonstoichiometry

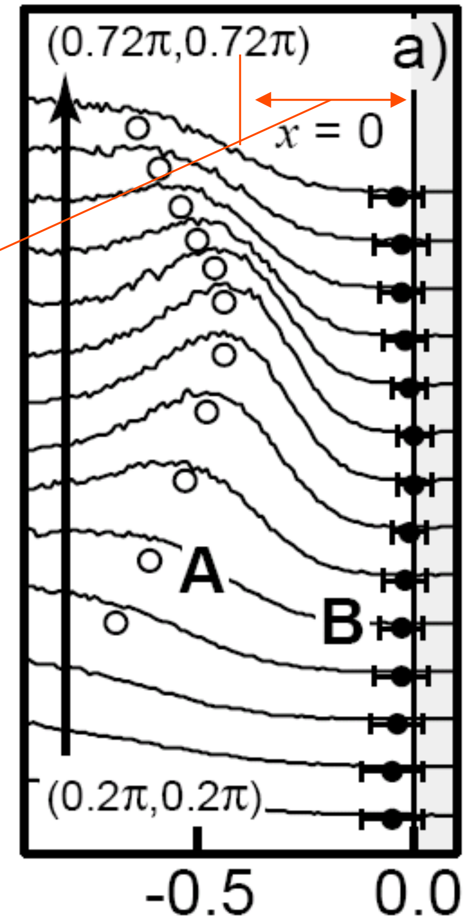
Fermi level pinned at top of lower charge transfer band




$Nd_2CuO_4$

Armitage et al, PRL 2002




$Ca_2CuO_2Cl_2$

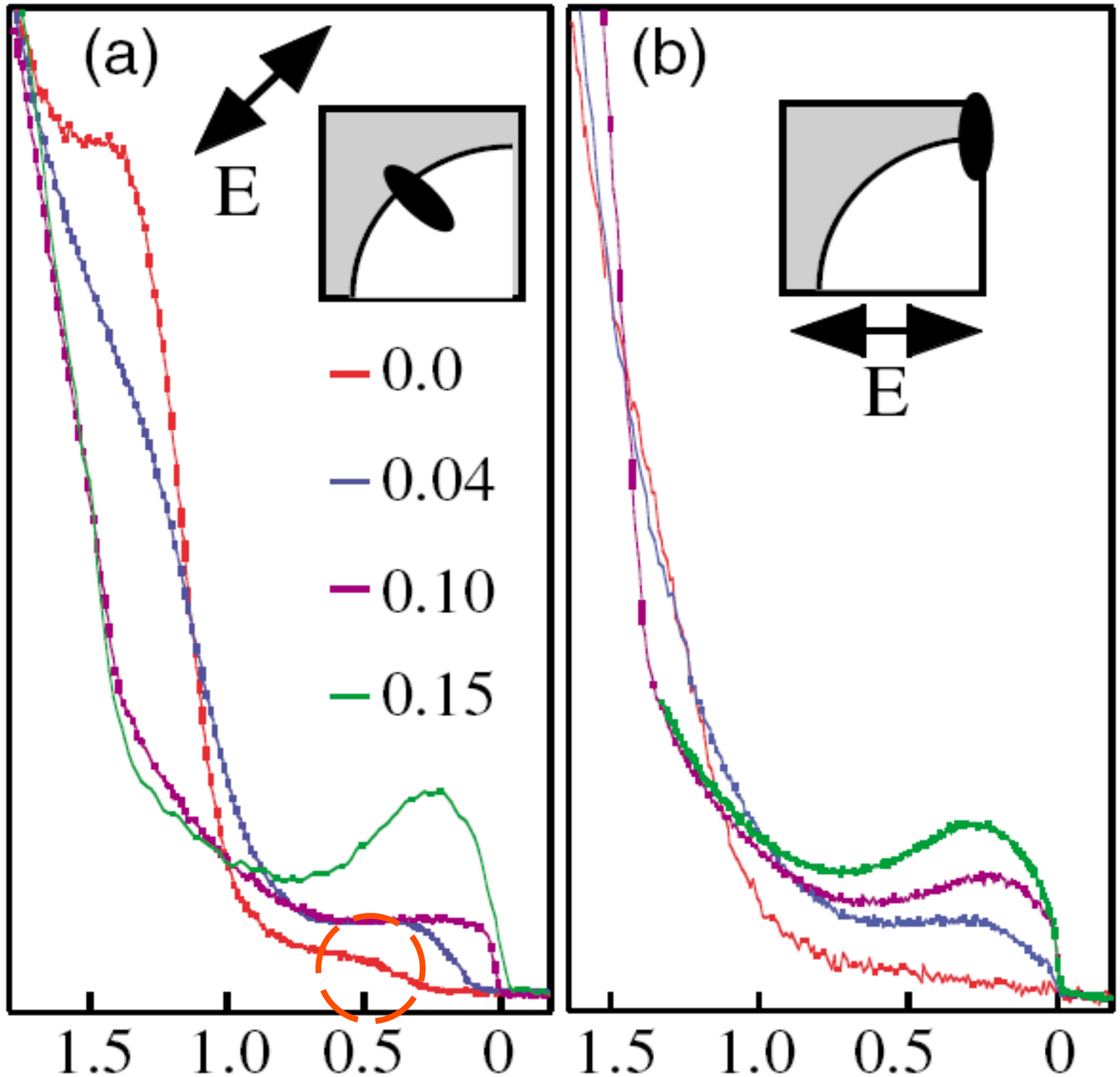
Shen et al, PRL 2004

# How does the CT gap collapse?

Along zone diagonal:

- Low energy peak moves from ~0.5eV at zero doping towards the Fermi level with increasing doping
- At zero doping

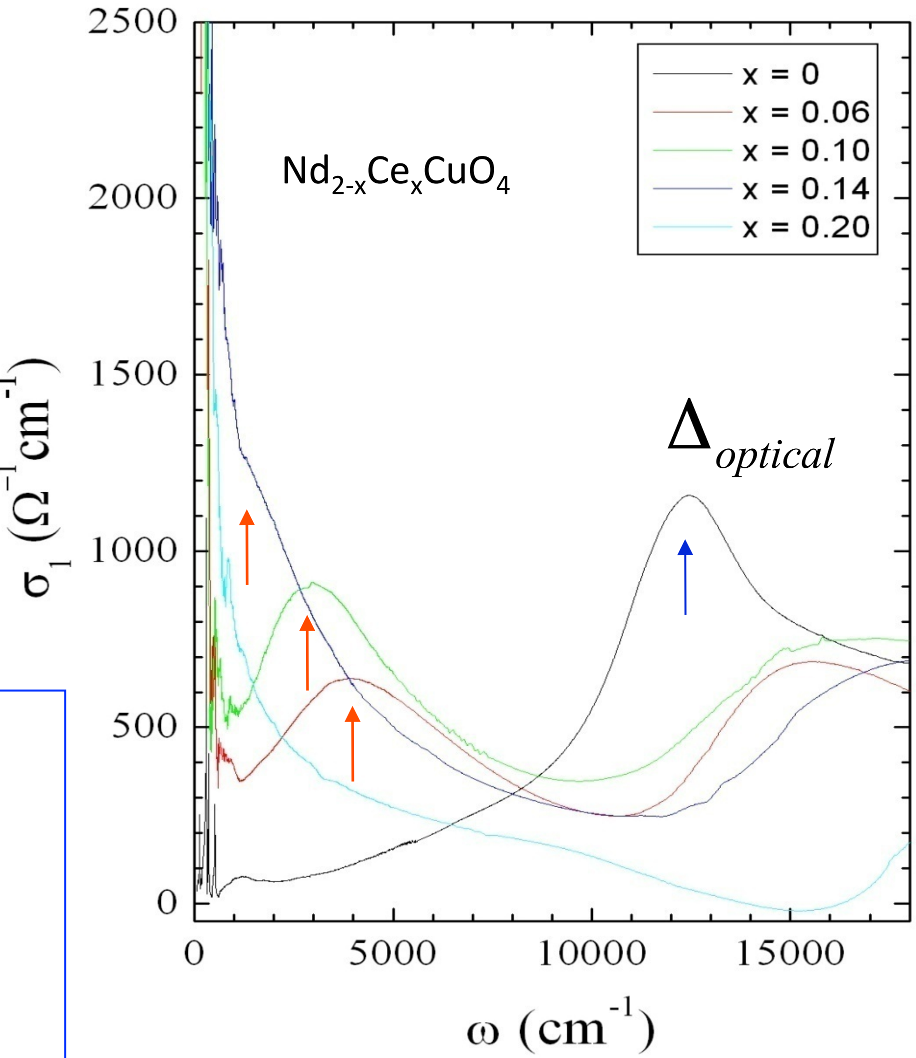
$$\Delta_{CT} \sim 0.5eV$$
$$\Delta_{optical} \sim 1.5eV$$




NP Armitage et al, PRL 2002

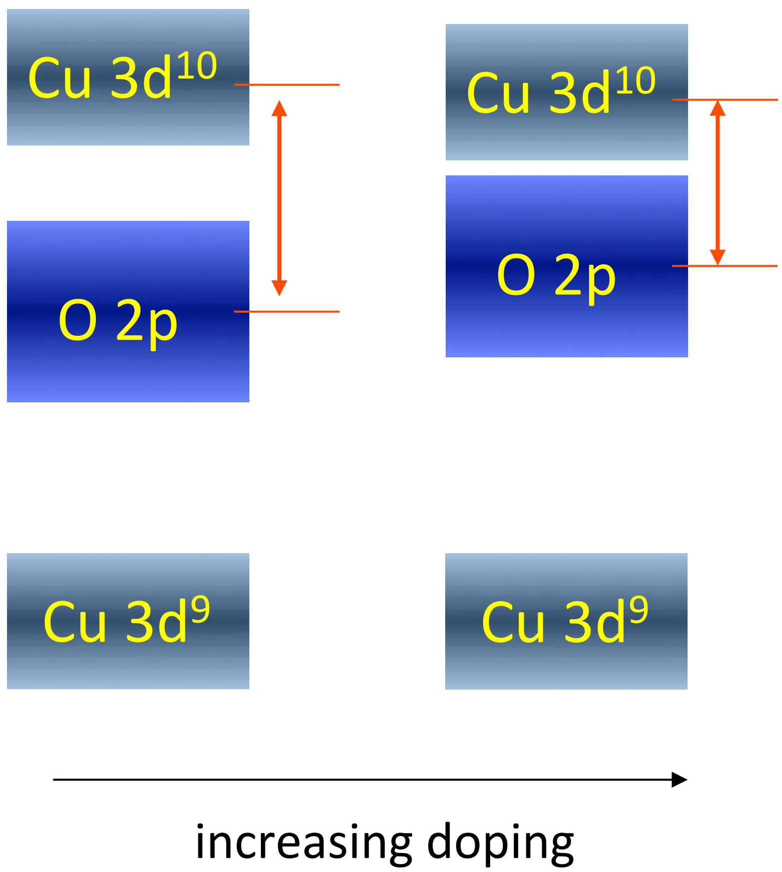
# Doping Evolution of Mid-infrared Peak

Onose et al, PRL 2001
NL Wang et al, PRB 2006




A mid-infrared peak at ~0.5eV at low doping moves towards zero energy with increasing doping

# Summary: CT Gap drops with doping



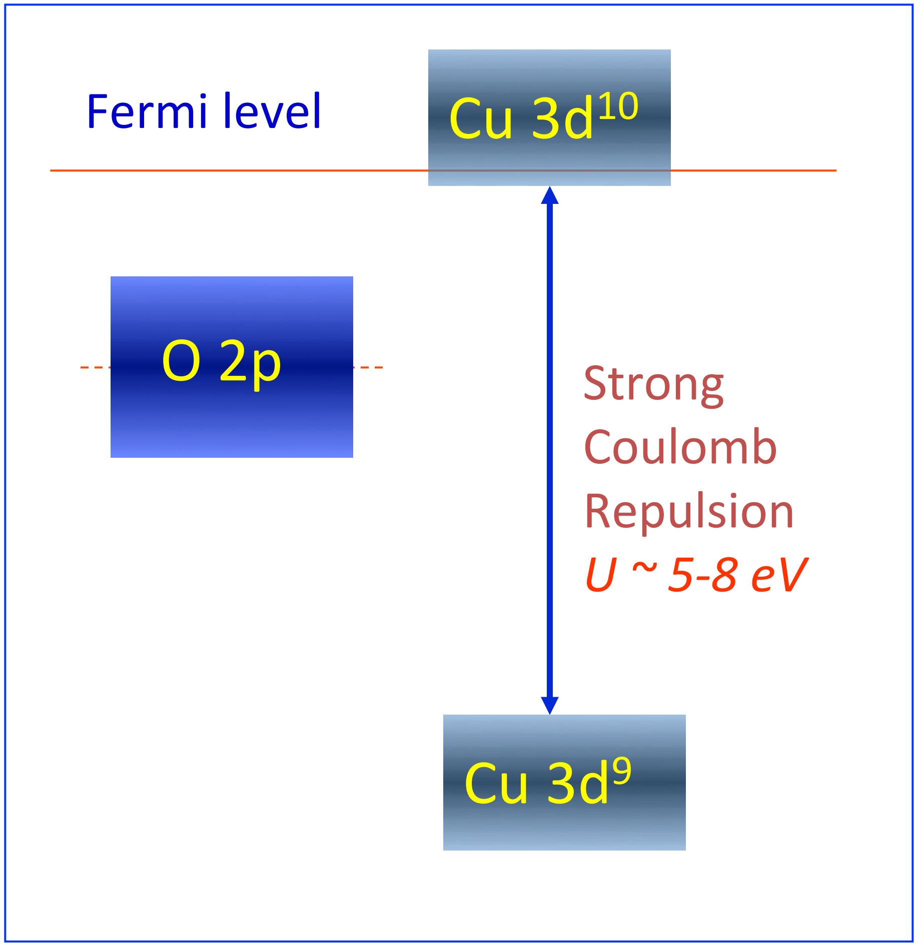

- Both ARPES and optics show that doping reduces the CT gap

- Closing of the CT gap indicates that the O 2p band will move towards Cu $3d^{10}$ band with doping

# What forces drive O 2p and Cu $3d^{10}$ bands closer?

Coulomb screening reduces *U*, driving Cu $3d^{10}$ band downwards

Coulomb repulsion between O 2p and doped Cu $3d^{10}$ electrons drives the O 2p band upwards



# Driving force for the upward moving of O 2p band

Coulomb repulsion between O 2p and Cu 3d electrons

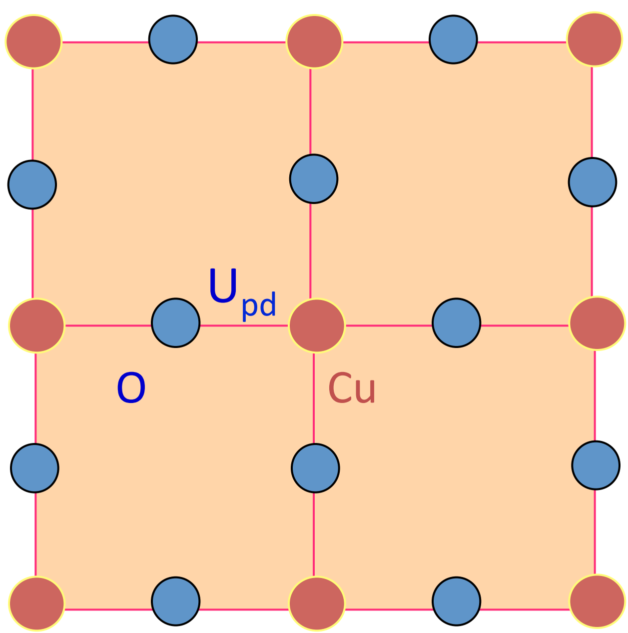
$$H_I = U_{pd} \sum_{\langle il \rangle} n_{ip} n_{ld}$$

Doping concentration

$$\Delta H_I = U_{pd} \sum_{\langle il \rangle} n_{ip} x$$

$$\varepsilon_p \rightarrow \varepsilon_p + 2xU_{pd}$$

Electron doping to Cu 3d states will on average shift the energy level of O 2p states




$$U_{pd} \sim 1 - 2\ eV$$

$$\Delta\varepsilon_p \sim 0.3 - 0.6\ eV \quad \text{if } x = 0.15$$

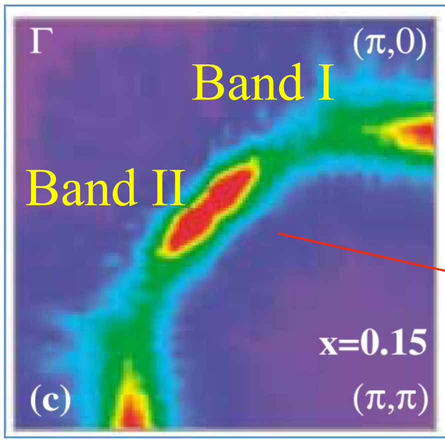
$$\Delta_{CT} \sim 0.5\ eV$$

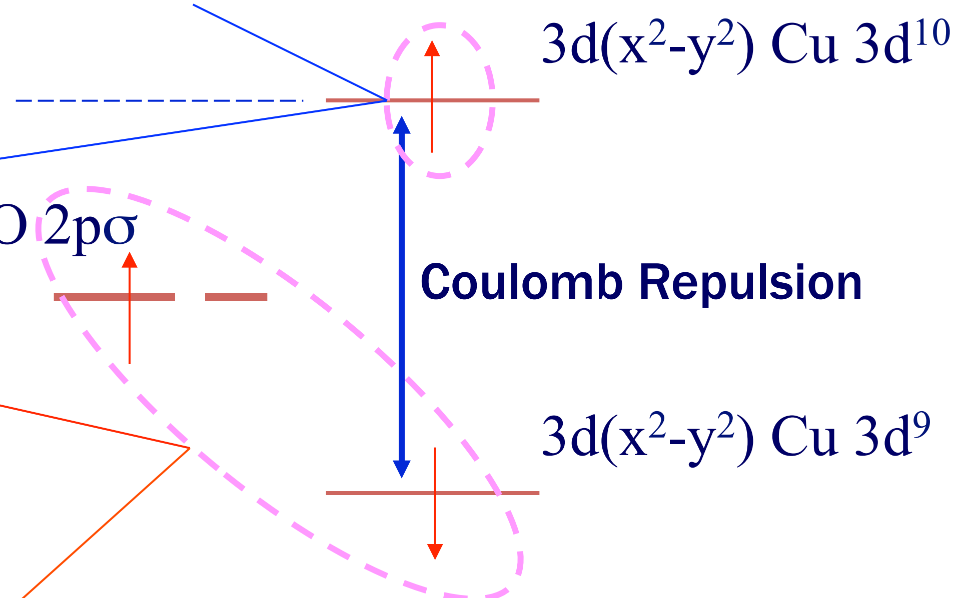
# How to model this system?

$e_i$ : doublon
$d_{i\sigma}$ : spinon
$h_i$ : Z-R singlet

t-J model

$$H = \sum_{ij\sigma} t_{ij}^{e} e_i^{+} d_{i\sigma} d_{j\sigma}^{+} e_j + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

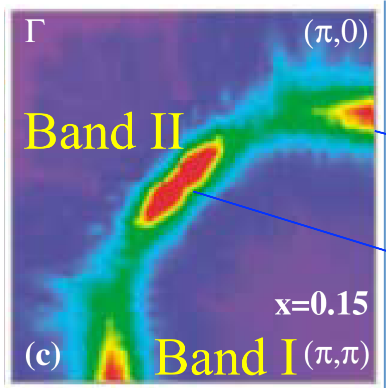



t-J model

$$H = \sum_{ij\sigma} t_{ij}^{h} d_{i\sigma}^{+} h_i h_j^{+} d_{j\sigma} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

O 2p hole binds with a $Cu^{2+}$ spin to form a Zhang-Rice singlet




# Hybridized Two Bands

Zhang-Rice singlet — Holon band

Cu $3d^{10}$ — Doublon band

Cu $3d^{9}$ — Spin Exchange

Hybridization between holon & doublon bands →

Holon-Doubleon Coulomb attraction →

$$H = \sum_{ij\sigma} \left( t_{ij}^{h} d_{i\sigma}^{+} h_i h_j^{+} d_{j\sigma} + t_{ij}^{e} e_i^{+} d_{i\sigma} d_{j\sigma}^{+} e_j \right) + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$
$$+ \sum_{ij\sigma} \left( \sigma t_{ij} d_{i\sigma}^{+} d_{j\bar{\sigma}}^{+} h_j e_i + h.c. \right) + \sum_i \left( \varepsilon_e e_i^{+} e_i + \varepsilon_h h_i^{+} h_i \right)$$
$$- V_{pd} \sum_{\langle ij \rangle} h_i^{+} h_i e_j^{+} e_j$$

Constraint

$$\sum_{\sigma} d_{i\sigma}^{+} d_{i\sigma} + e_i^{+} e_i + h_i^{+} h_i = 1$$

T Xiang et al, Phys Rev B **79**, 014524 (2009)  Luo, Xiang, PRL **94** (2005) 027001

# Symmetric Limit: $t_{ij}^h = t_{ij}^e = t_{ij}$

Two bands

$$H = \sum_{ij\sigma} \left( t_{ij}^h d_{i\sigma}^+ h_i h_j^+ d_{j\sigma} + t_{ij}^e e_i^+ d_{i\sigma} d_{j\sigma}^+ e_j \right) + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$
$$+ \sum_{ij\sigma} \left( \sigma t_{ij} d_{i\sigma}^+ d_{j\bar{\sigma}}^+ h_j e_i + h.c. \right) + \sum_i \left( \varepsilon_e e_i^+ e_i + \varepsilon_h h_i^+ h_i \right)$$
$$- V_{pd} \sum_{\langle ij \rangle} h_i^+ h_i e_j^+ e_j$$

$$c_{i\sigma} = \sigma h_i^+ d_{i\sigma} + d_{i\bar{\sigma}}^+ e_i$$

One-band
t-U-J Model

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$U = \varepsilon_e + \varepsilon_h - 4V_{pd} \left( \left\langle e_i^+ e_i \right\rangle + \left\langle h_i^+ h_i \right\rangle \right) \approx \Delta_{CT}^0 - 4xV_{pd}$$

T Xiang et al, Phys Rev B **79**, 014524 (2009)   Luo, Xiang, PRL **94** (2005) 027001

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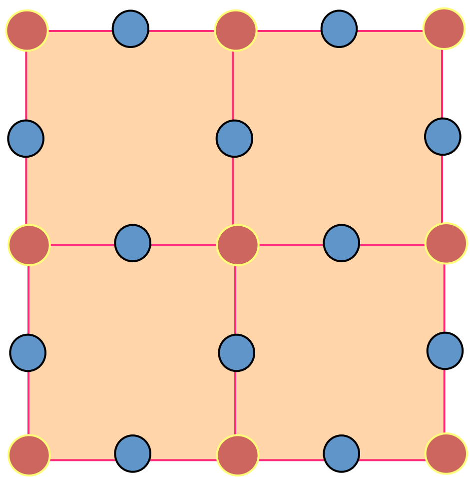
# How do electrons hop from one layer to another?

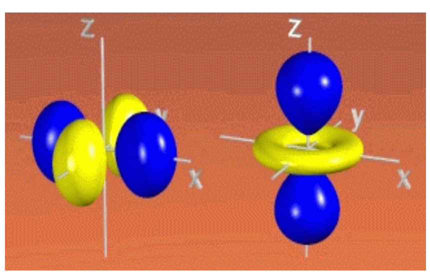
T Xiang, J M Wheatley, PRL 77,4632 (1996)



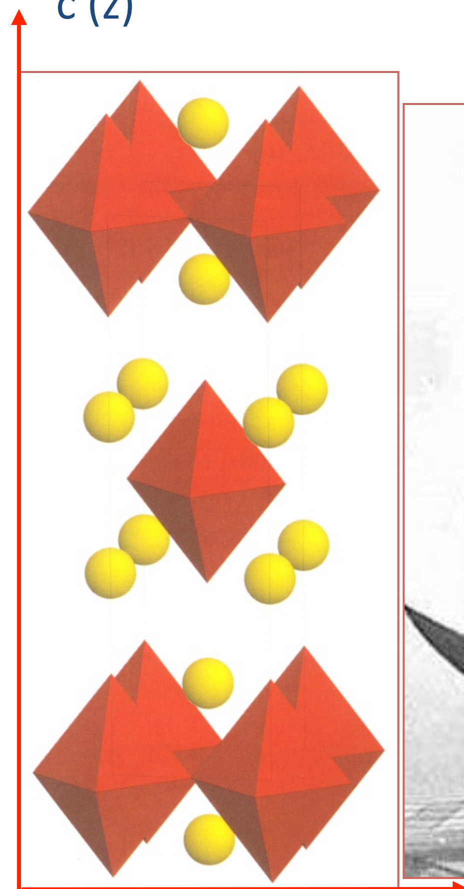
Cu

O

$CuO_2$ plane

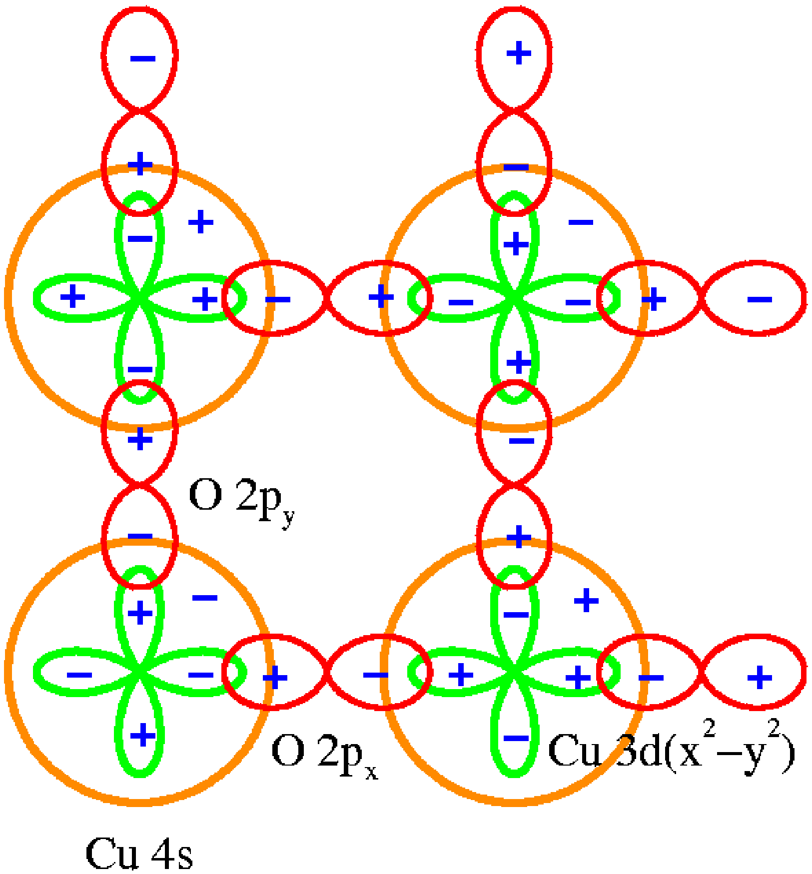


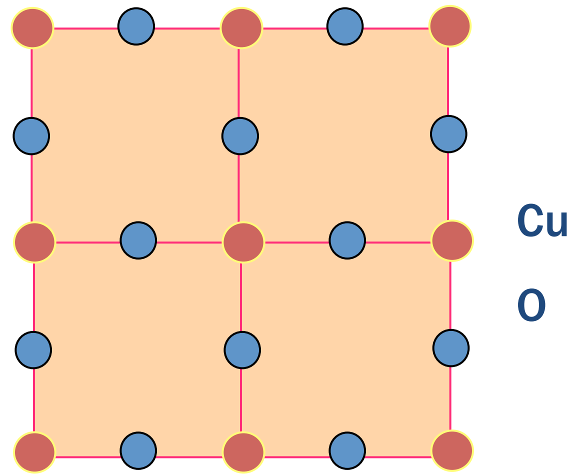

c (z)



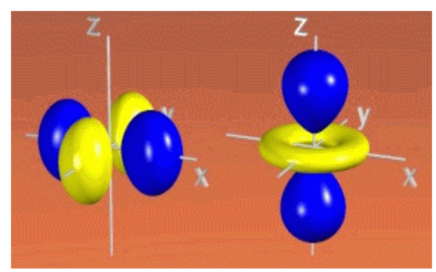
a,b (x,y)

# How do electrons hop from one layer to another?



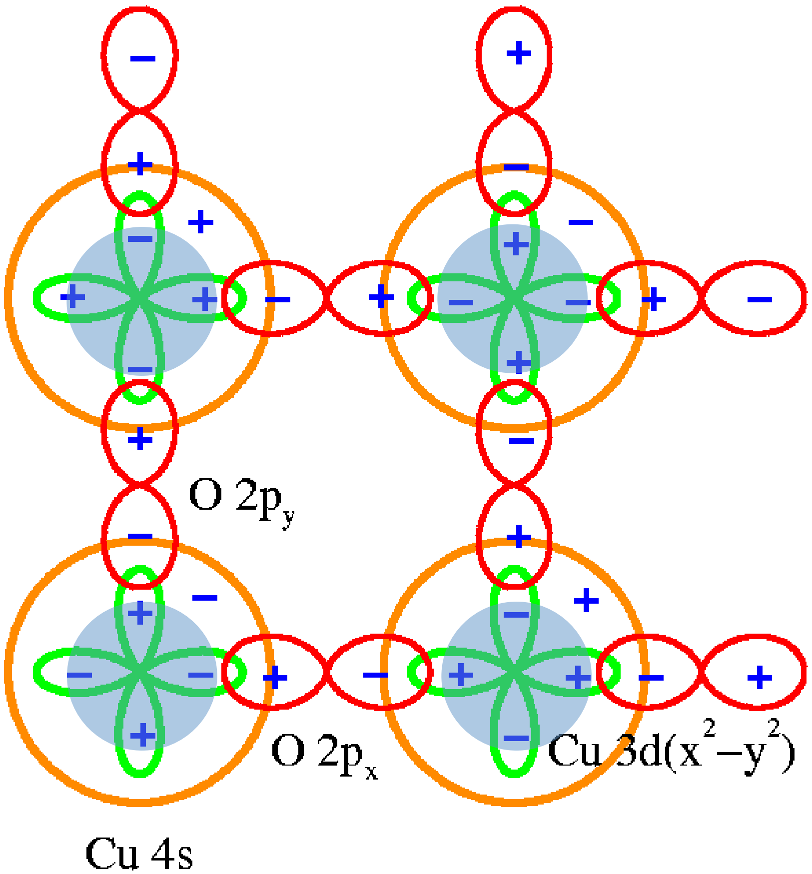

$CuO_2$ plane

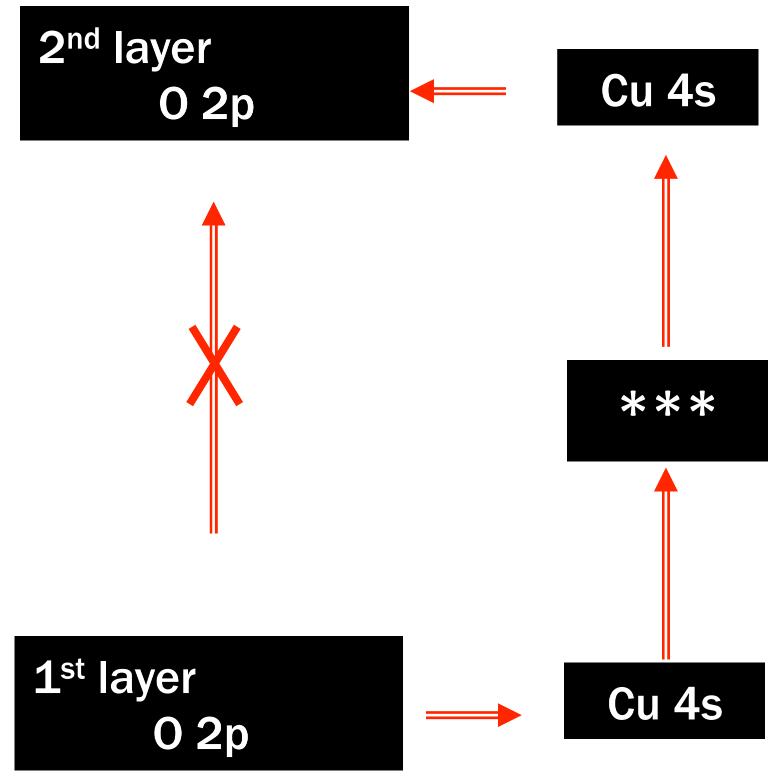


# Interlayer Hopping Integral:

$$t_z \propto t_\perp \left(\cos k_x - \cos k_y\right)^2$$

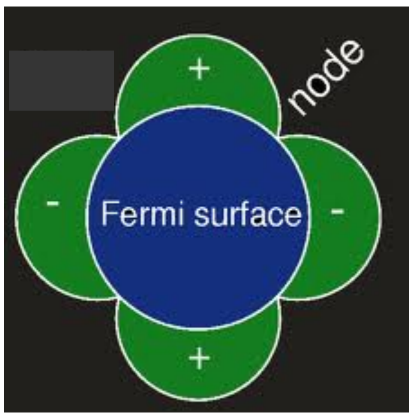
$$t_z \sim \left\langle O_{2p} \,|\, Cu_{4s} \right\rangle_2 \left\langle Cu_{4s} \,|\, * \right\rangle \left\langle * \,|\, Cu_{4s} \right\rangle \left\langle Cu_{4s} \,|\, O_{2p} \right\rangle_1$$



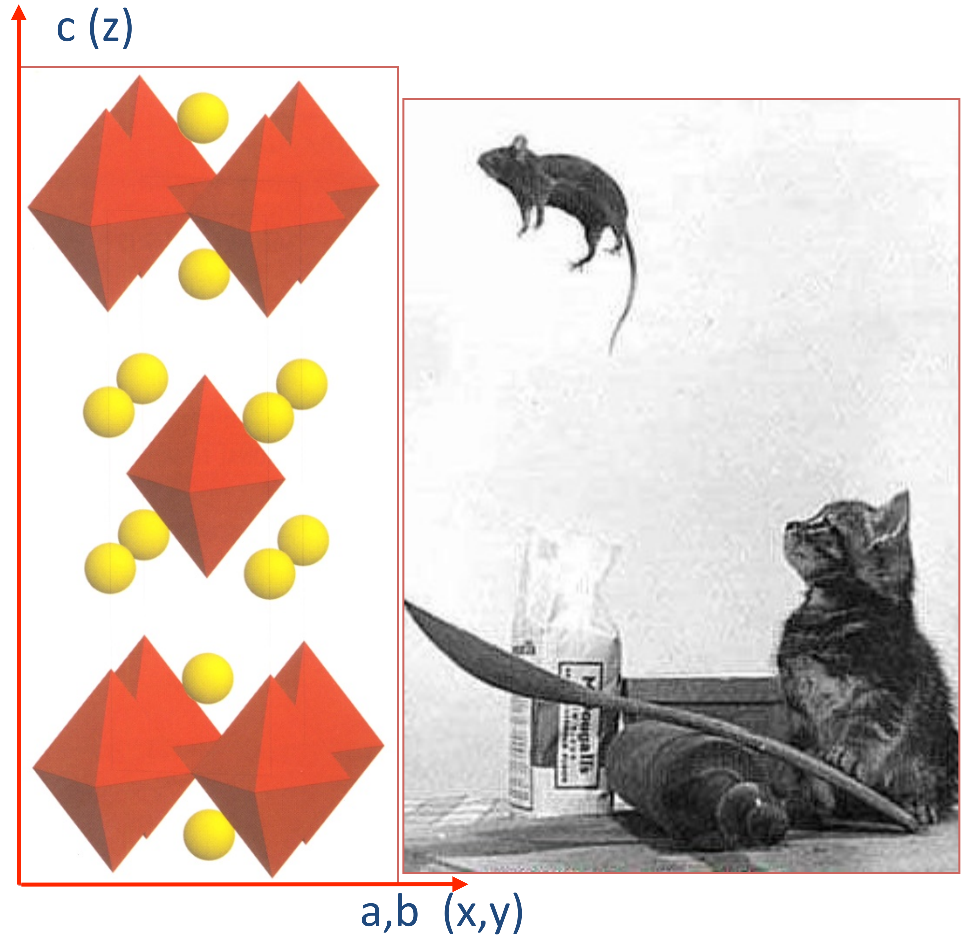



# Interlayer hopping depends strongly on the in-plane momentum

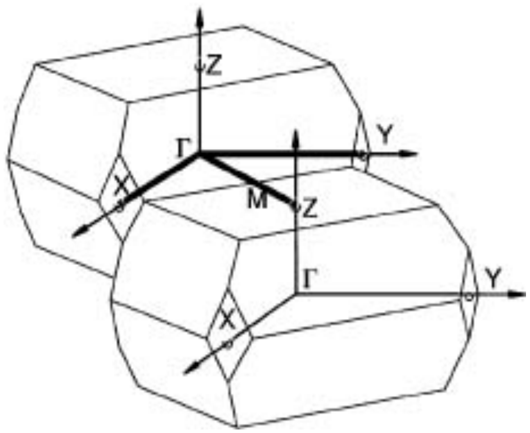
$$t_z \propto t_\perp \left(\cos k_x - \cos k_y\right)^2$$




c-axis hopping vanishes along two diagonal directions

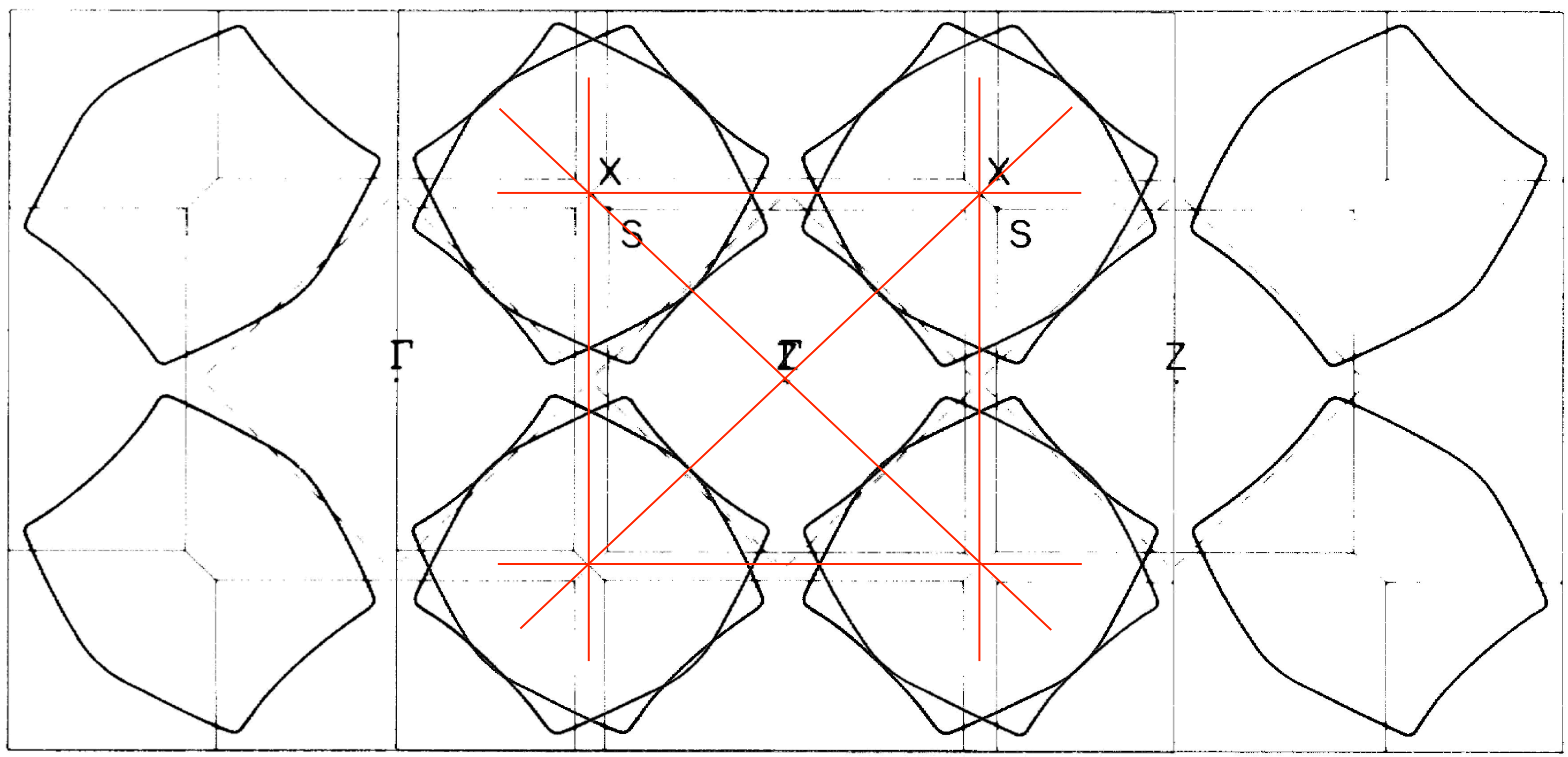



T Xiang, J M Wheatley, PRL **77**,4632 (1996)



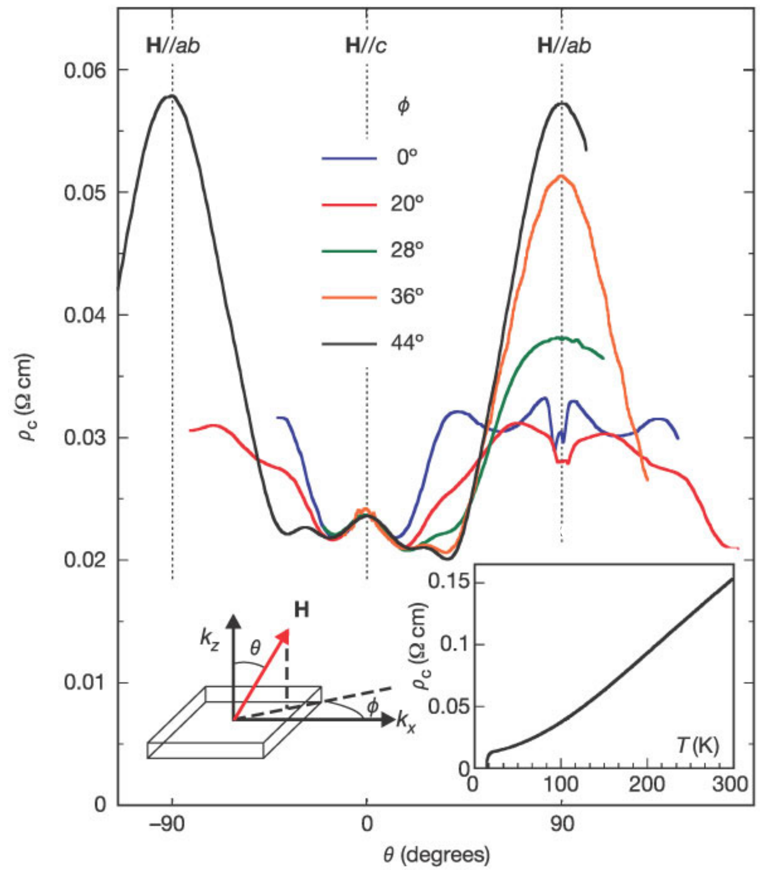

# Fermi Surface of $La_{2-x}Sr_xCuO_4$

$$t_z \propto t_\perp \left(\cos k_x - \cos k_y\right)^2 \cos\frac{k_x}{2}\cos\frac{k_y}{2}$$

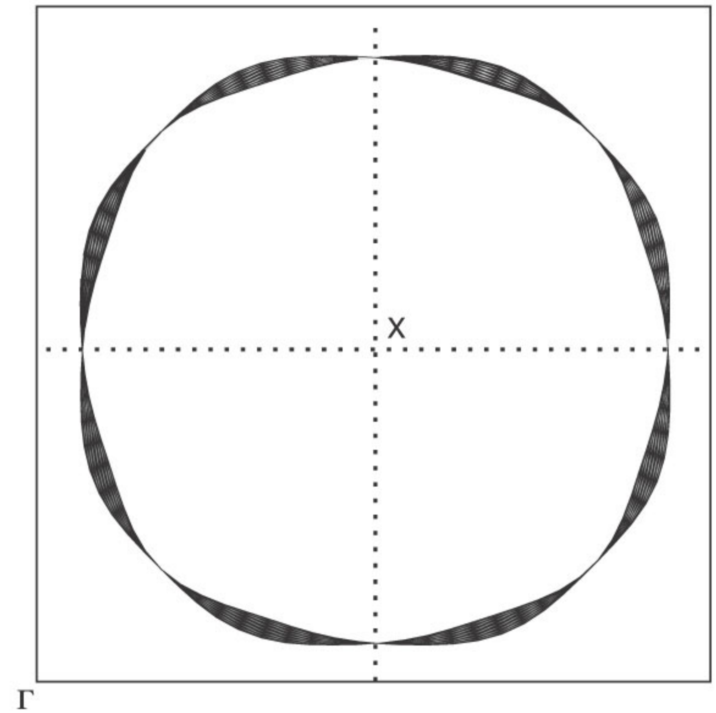


# Coherent 3D Fermi surface measured by Polar Angular Magnetoresistance Oscillation

Hussey et al, Nature 425, 814 (03)

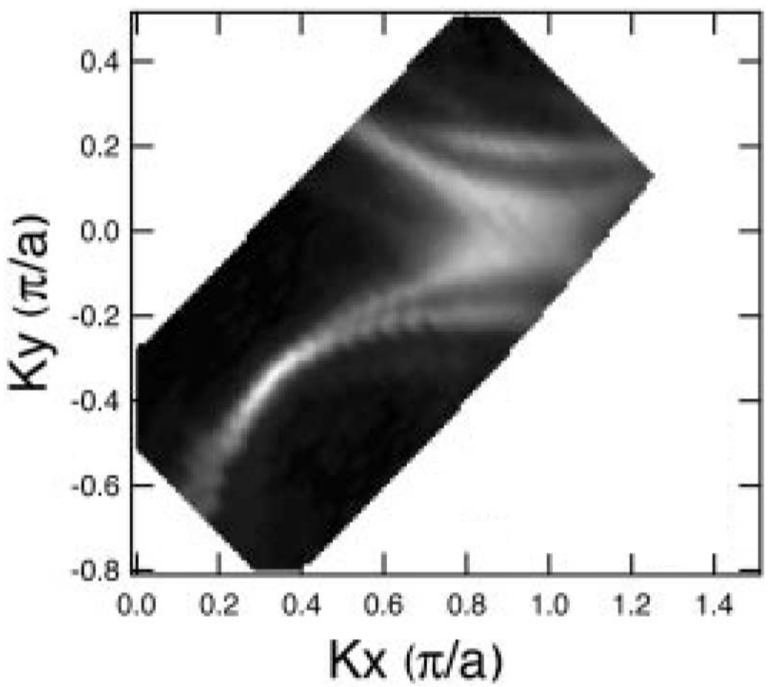



**Polar AMRO, overdoped Tl2201**



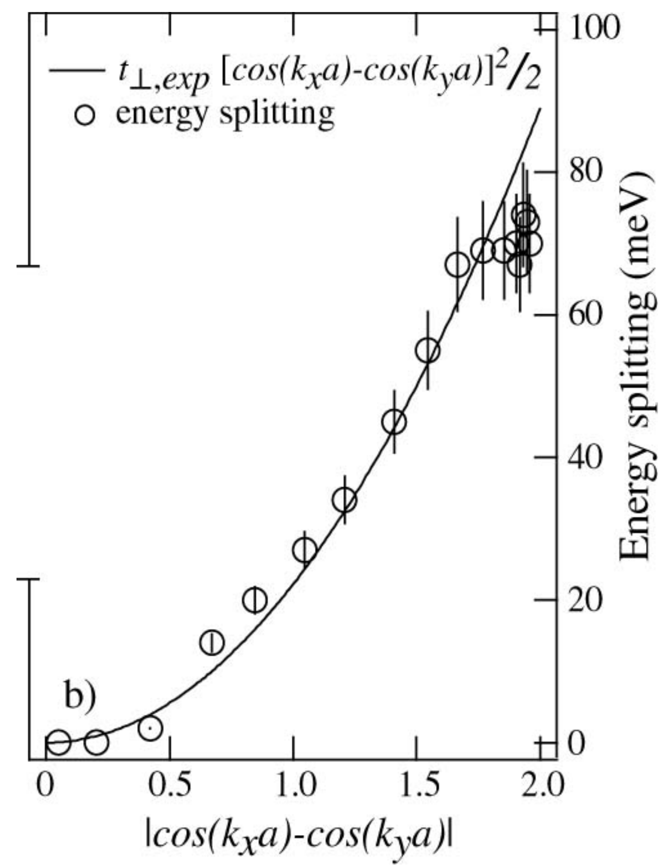

**Projection of the FS onto the ab-plane**

# ARPES for the bilayer split of Bi2212




Bogdanov et al, PRB **64**, 180505 (01)

$t_{\perp \exp} = 44 \pm 5 meV$

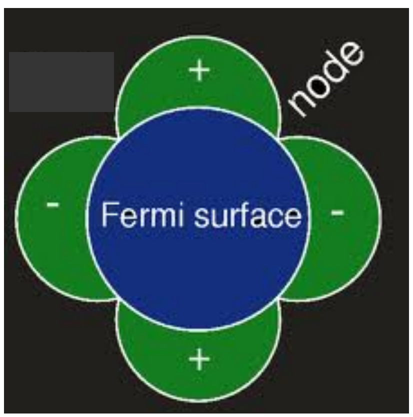



D L Feng et al, PRL **86**, 5550 (01)

# Interplay between anistropic c-axis hopping and d-wave superconducting/pseudo-gap

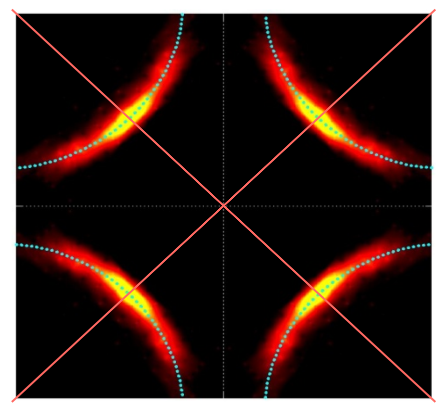
- No gap for the excitations along diagonals: metallic
- Electrons whose in-plane momenta are on the two diagonals cannot hop along the c-axis: semiconducting

$$t_z \propto t_\perp \left(\cos k_x - \cos k_y\right)^2$$



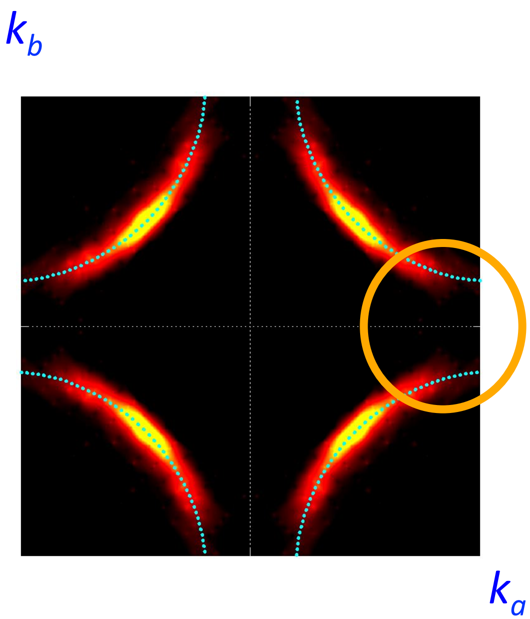

c-axis hopping vanishes along two diagonal directions

$$\Delta \propto \Delta_0 \left(\cos k_x - \cos k_y\right)$$



Superducting/pseudo-gap vanishes along two diagonals

# Universal Scaling Law of the c-axis Resistivity




**Pseudogap Δ is the only control parameter of low energy excitations**

↓

**Universal scaling law**

$$\rho_c(T) = \alpha_c g\left(\frac{T}{\Delta}\right)$$

Su, Luo, Xiang, PRB (2006）

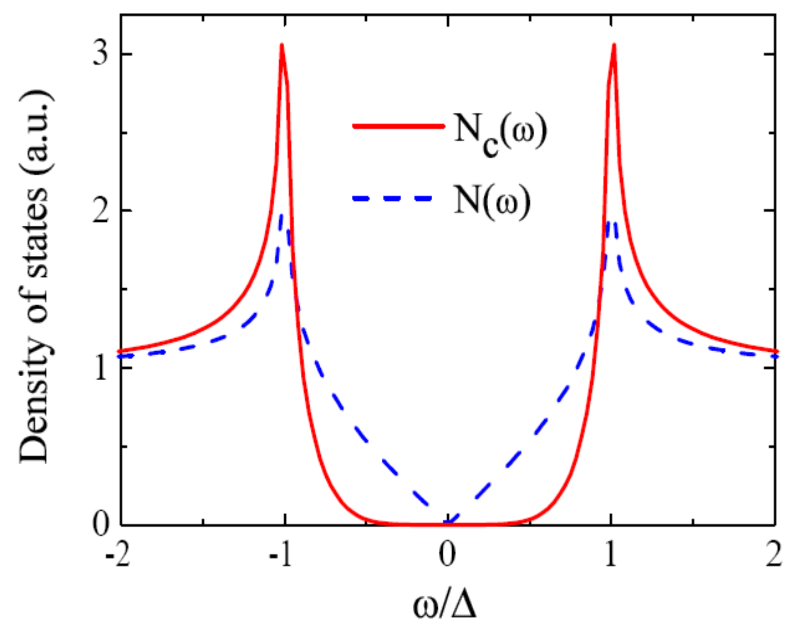
# Scaling Function

$$\sigma_c \sim \frac{1}{\Gamma}\int_{-\infty}^{\infty} d\omega \frac{\partial f(\omega)}{\partial \omega}\left\langle t_z^2(k)\rho(\omega,k)\right\rangle_{F.S} = \frac{1}{\Gamma}\int_{-\infty}^{\infty} d\omega \frac{\partial f(\omega)}{\partial \omega} N_c(\omega)$$

$$N_c(\omega) = \left\langle t_z^2(k)\rho(\omega,k)\right\rangle_{FS} \approx N_0\delta(\omega-\Delta)$$

$$\rho_c(T) = \sigma_c^{-1}(T) \propto T\exp\left(\frac{\Delta}{T}\right)$$

$$g\left(\frac{T}{\Delta}\right) \approx \frac{T}{\Delta}\exp\left(\frac{\Delta}{T}\right)$$

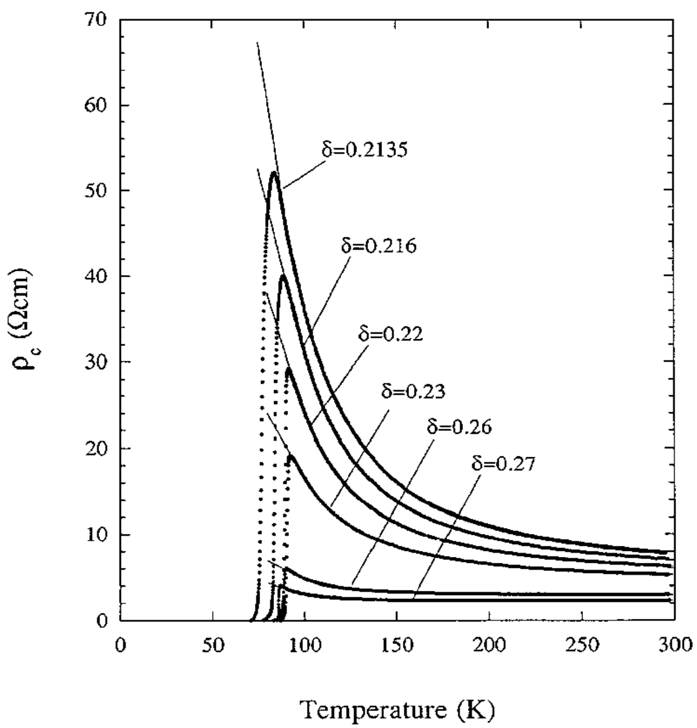


# Universal Scaling Law of the c-axis Resistivity

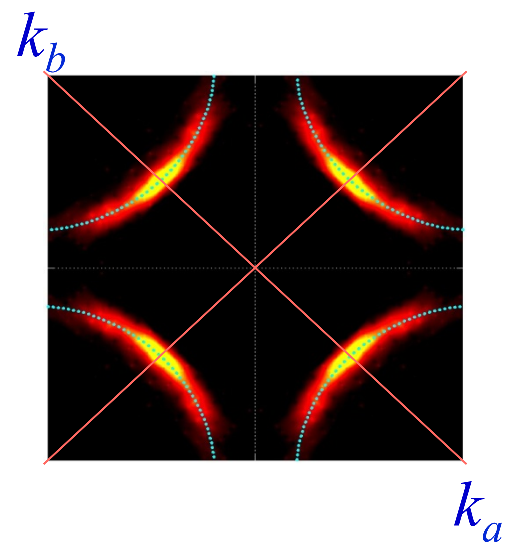
**c-axis resistivity** $$\rho_c(T) = \alpha_c g\left(\frac{T}{\Delta}\right)$$

$$g(x) \approx x \exp(1/x)$$

Bi2212




T. Watanabe et al. PRL 79, 2113 (1997)



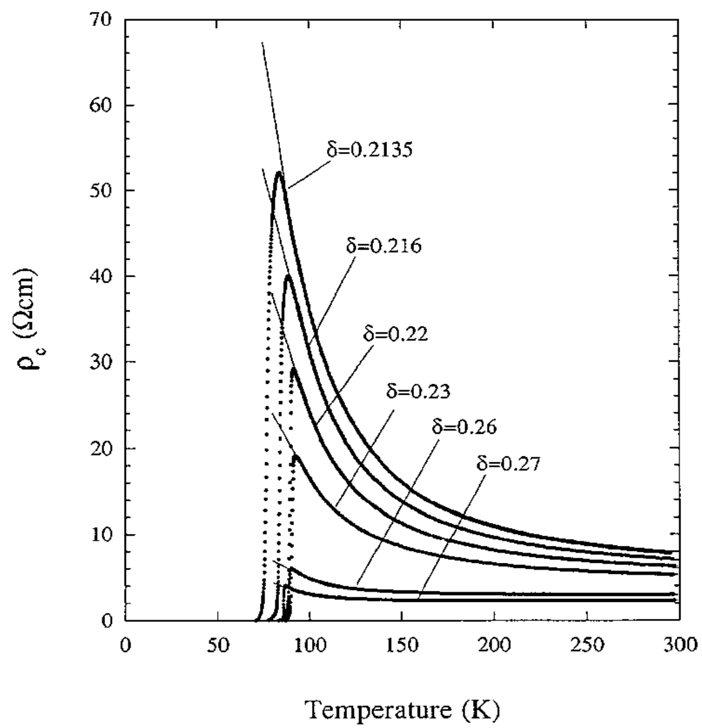

Su, Luo, Xiang, PRB **73**, 134510 (2006)

# Comparison with Experimental Data

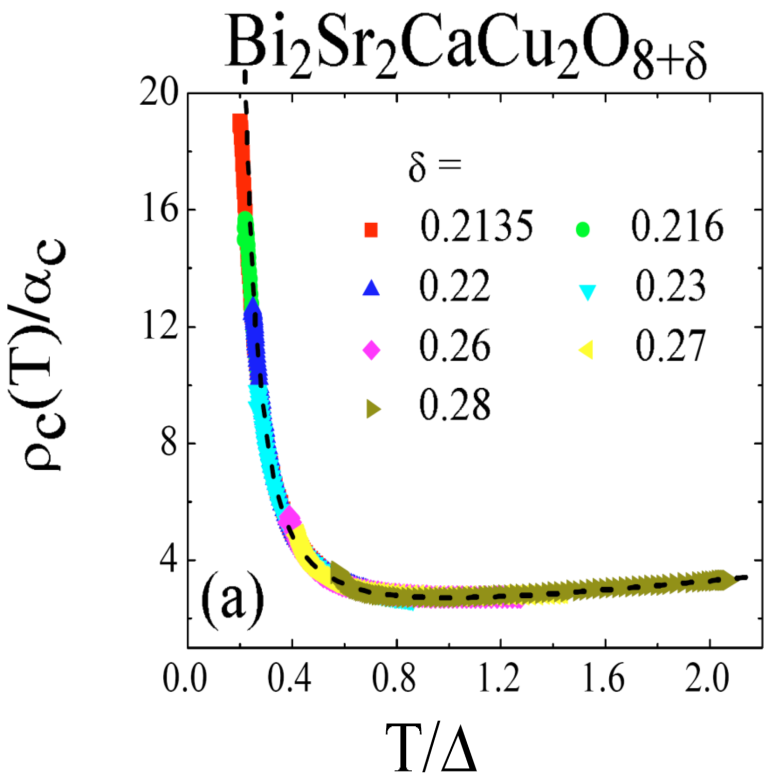
$$\rho_c(T) = \alpha_c g\left(\frac{T}{\Delta}\right)$$

$$g(x) \approx x\exp(1/x)$$

Bi2212




T. Watanabe et al. PRL 79, 2113 (1997)

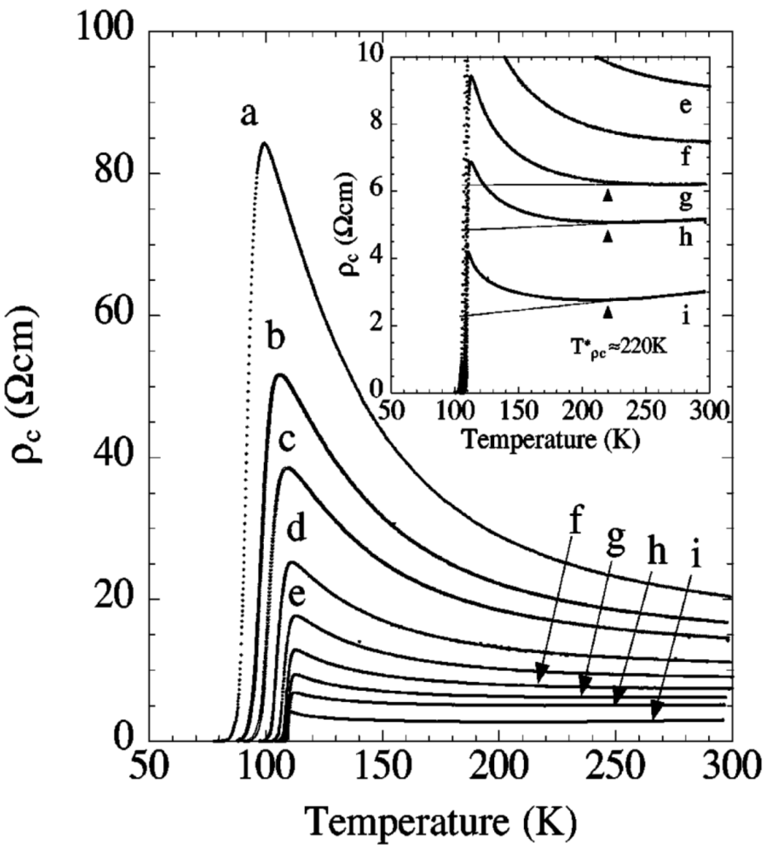


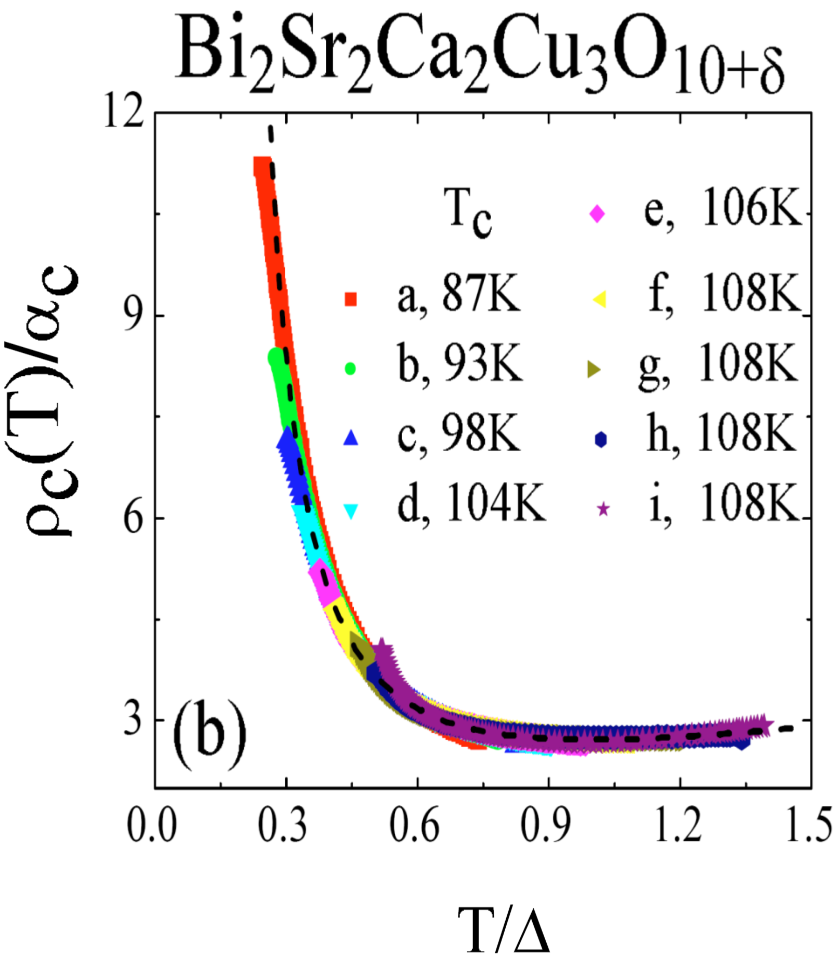
# Comparison with Experimental Data

$$\rho_c(T) = \alpha_c g\left(\frac{T}{\Delta}\right)$$

$$g(x) \approx x\exp(1/x)$$

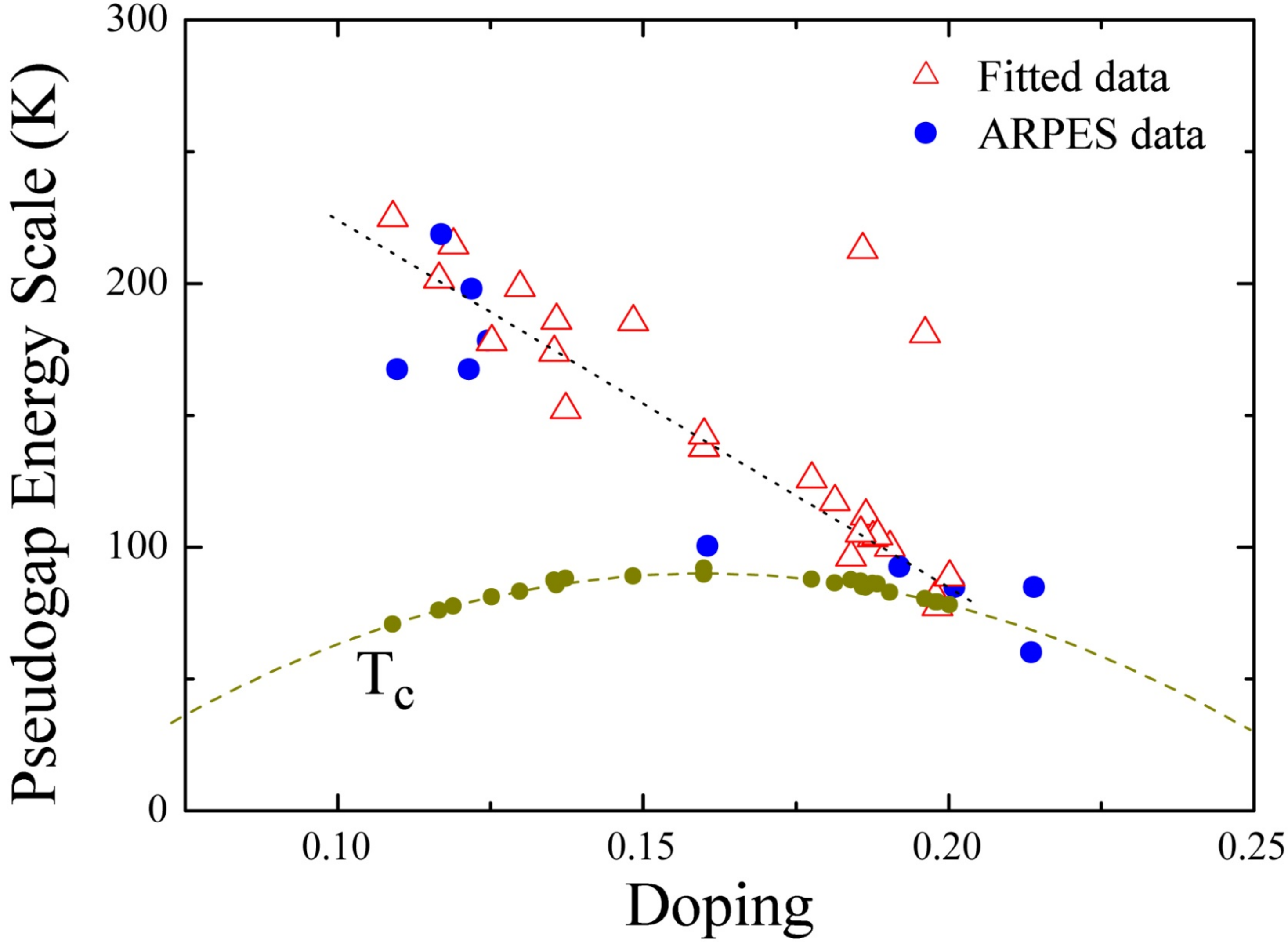
Bi2223




T. Fujii et al. PRB 66, 024507 (2002)

# Pseudogap


Fitted data
ARPES data
Pseudogap Energy Scale (K)
300
200
100
0
0.10
0.15
0.20
0.25
Doping
$T_c$

# c-axis Penetration Depth

$$\lambda_c^{-2} \sim \int d^3k v_c^2(k) \frac{\partial f(\lambda_k)}{\partial \lambda_k}$$

$$\sim \int d\omega \frac{\partial f(\omega)}{\partial \omega} \left\langle \cos^4 2\theta \rho(\omega, \theta) \right\rangle_{FS}$$

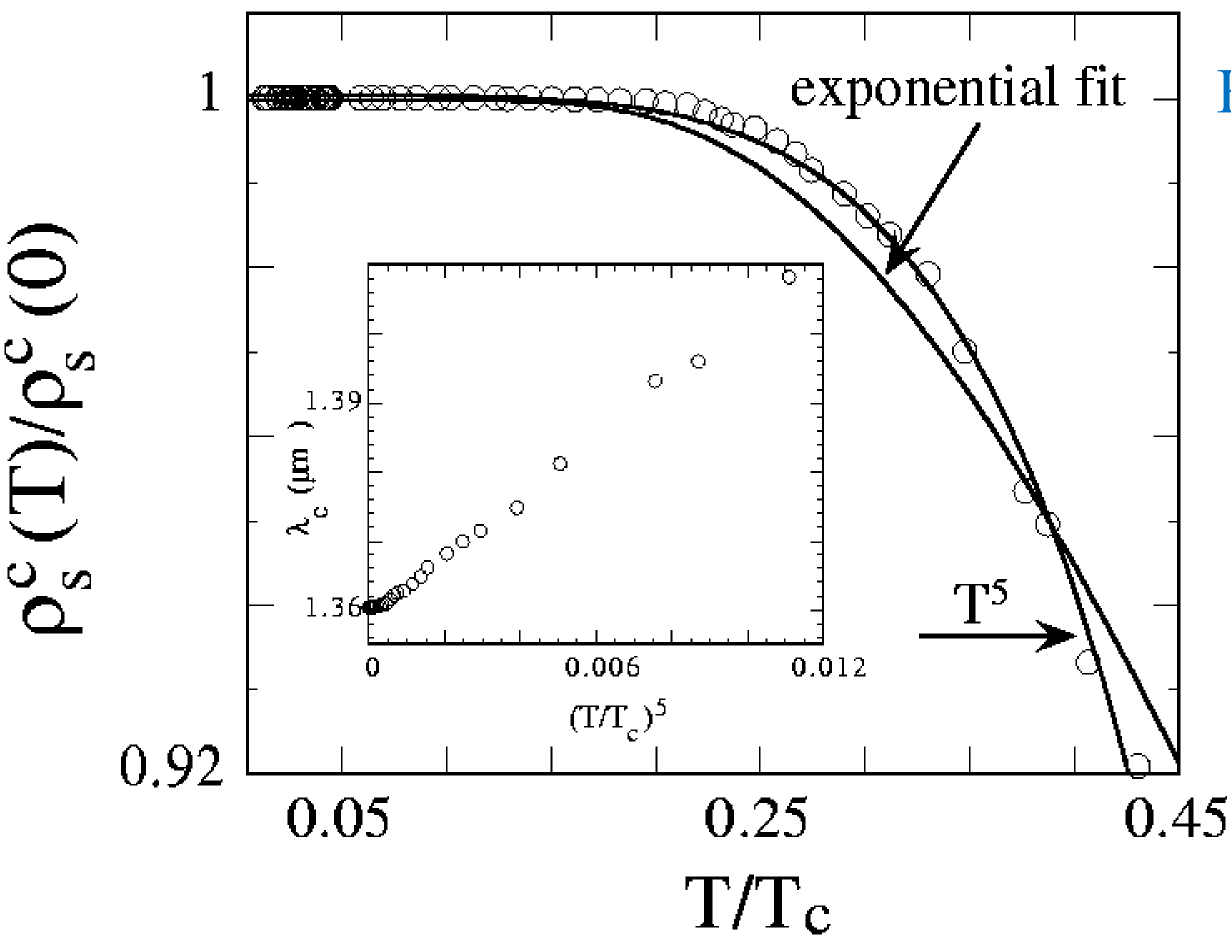
$$\Delta_\theta = \Delta \cos 2\theta$$

$$\lambda_c^{-2} \sim N(0) t_\perp^2 \left[ 1 - 450 \left( \frac{T}{\Delta_0} \right)^5 \right]$$

T. Xiang et al, PRL **77**, 4632 (96); Int J Mod Phys **12**, 1007 (98)

# c-axis Penetration Depth: $T^5$ Law

$$\lambda_c^{-2} \sim N(0)t_\perp^2\left[1-450\left(\frac{T}{\Delta_0}\right)^5\right]$$



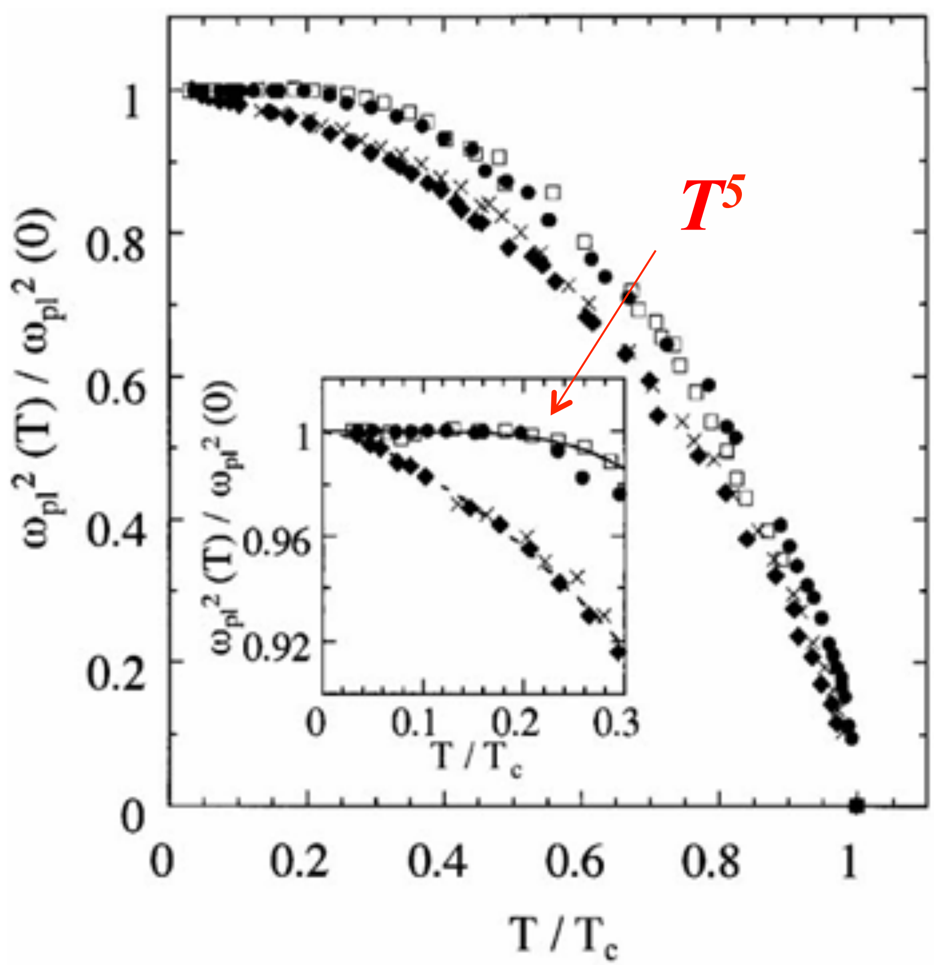

$HgBa_2CuO_4$

C. Panagopoulos et al
PRL **79**, 2320 (97)

# c-axis Penetration Depth: $T^5$ Law

$$\lambda_c^{-2} \sim N(0)\,t_\perp^2 \left[1 - 450\left(\frac{T}{\Delta_0}\right)^5\right]$$

$Bi_2Sr_2CaCu_2O_{8+x}$




M. B. Gaifullin, PRL **83**, 3928 (1999)

# Summary

- **Doped cuprates can be modeled by the t-J-U model**

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

**Hole doped cuprates:** $U \rightarrow \infty$

**Electron doped cuprates: smaller U**

- **The interlayer hopping is anisotropic and described by**

$$t_z \propto t_{\perp} \left( \cos k_x - \cos k_y \right)^2$$