# Consistent Picture of Magnetic Gap Collapse in $Nd_{2-x}Ce_xCuO_4$ (NCCO), Comparing ARPES and Resonant Inelastic X-ray Scattering (RIXS) Spectra

**R.S. Markiewicz****

***Northeastern University, Boston***

***** In collaboration with A. Bansil and Z. Hasan***

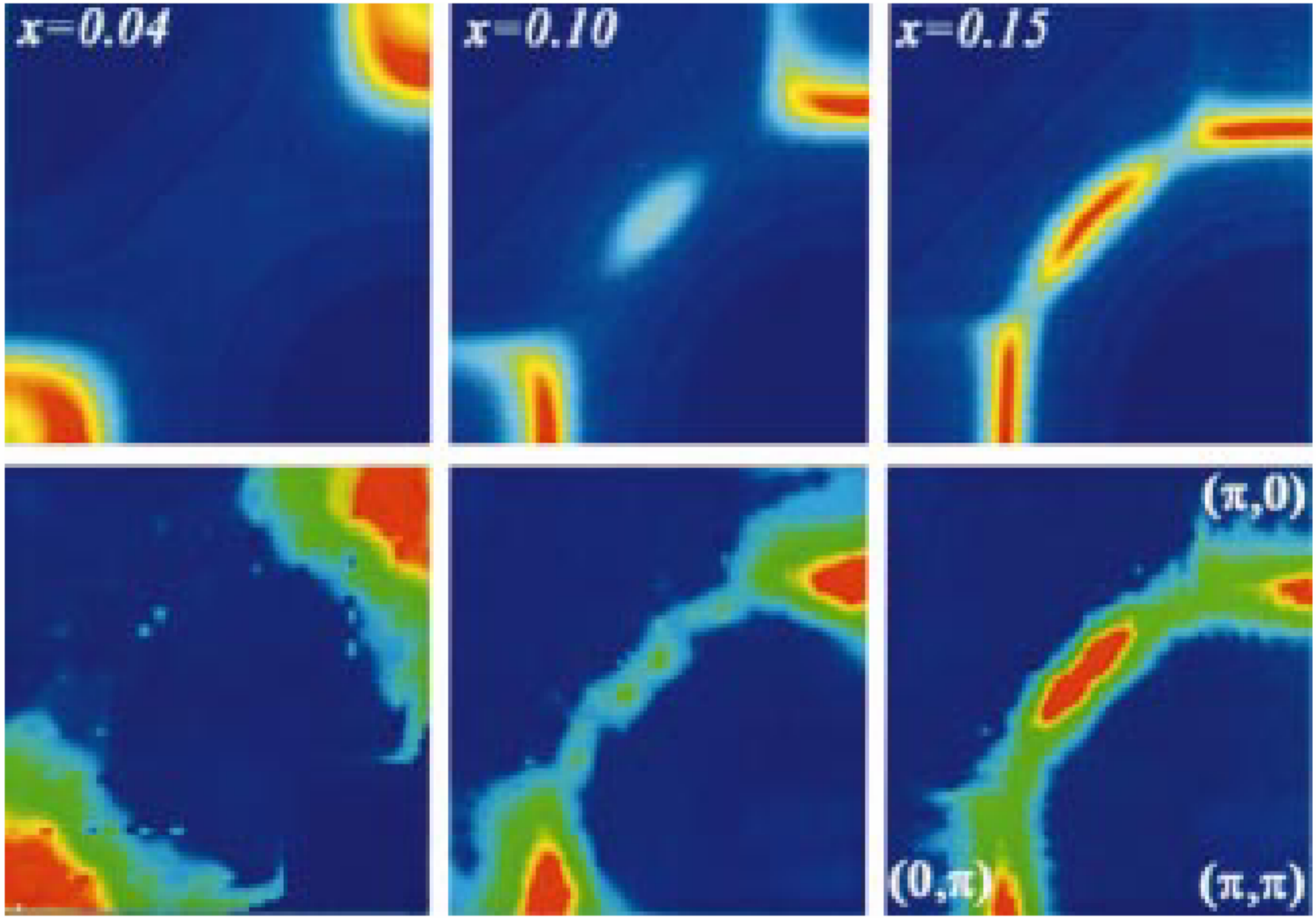
# Outline

- **ARPES in NCCO: Mott Gap Collapse?**
- **Multiband RIXS**
- **Application to NCCO**

# NCCO

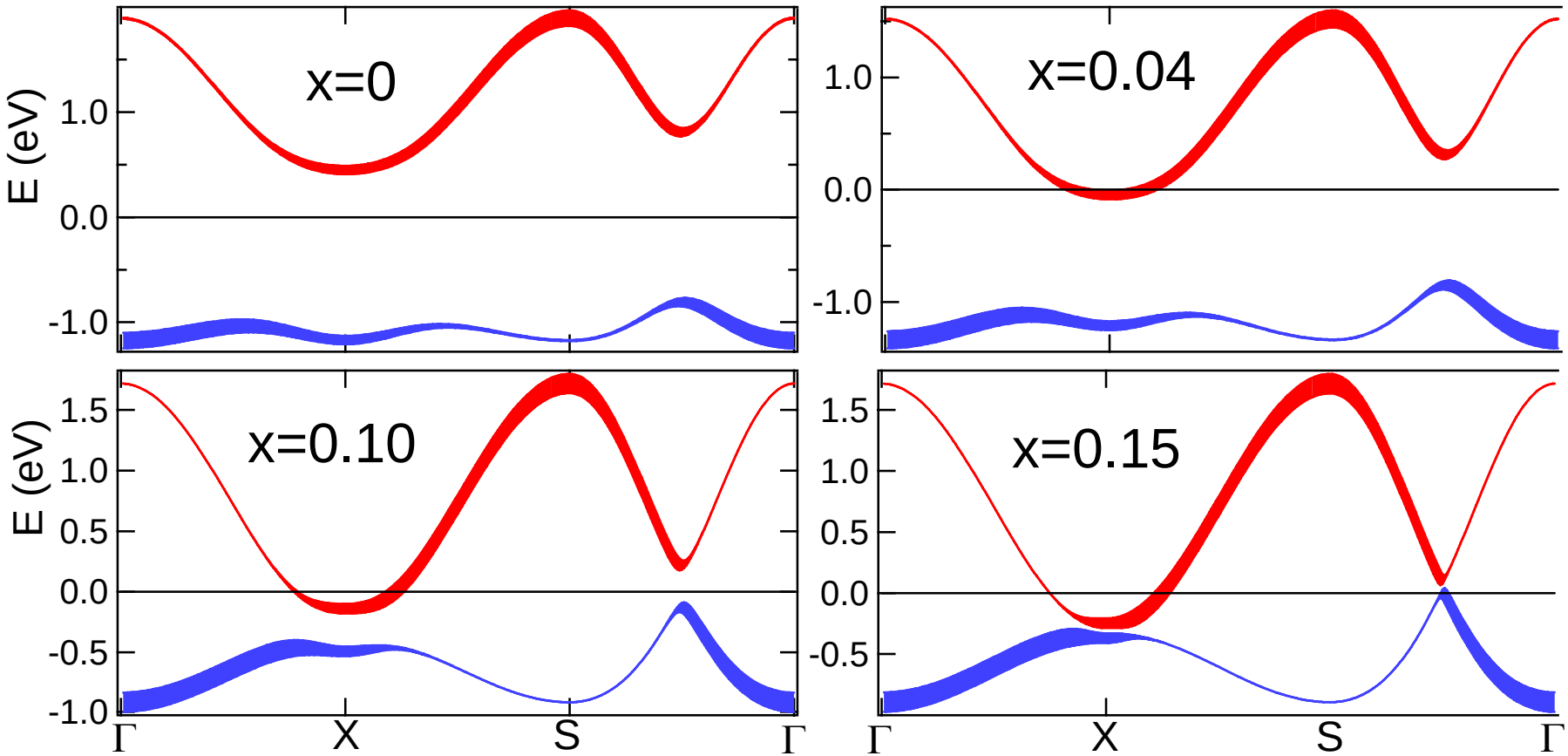
T:

E:



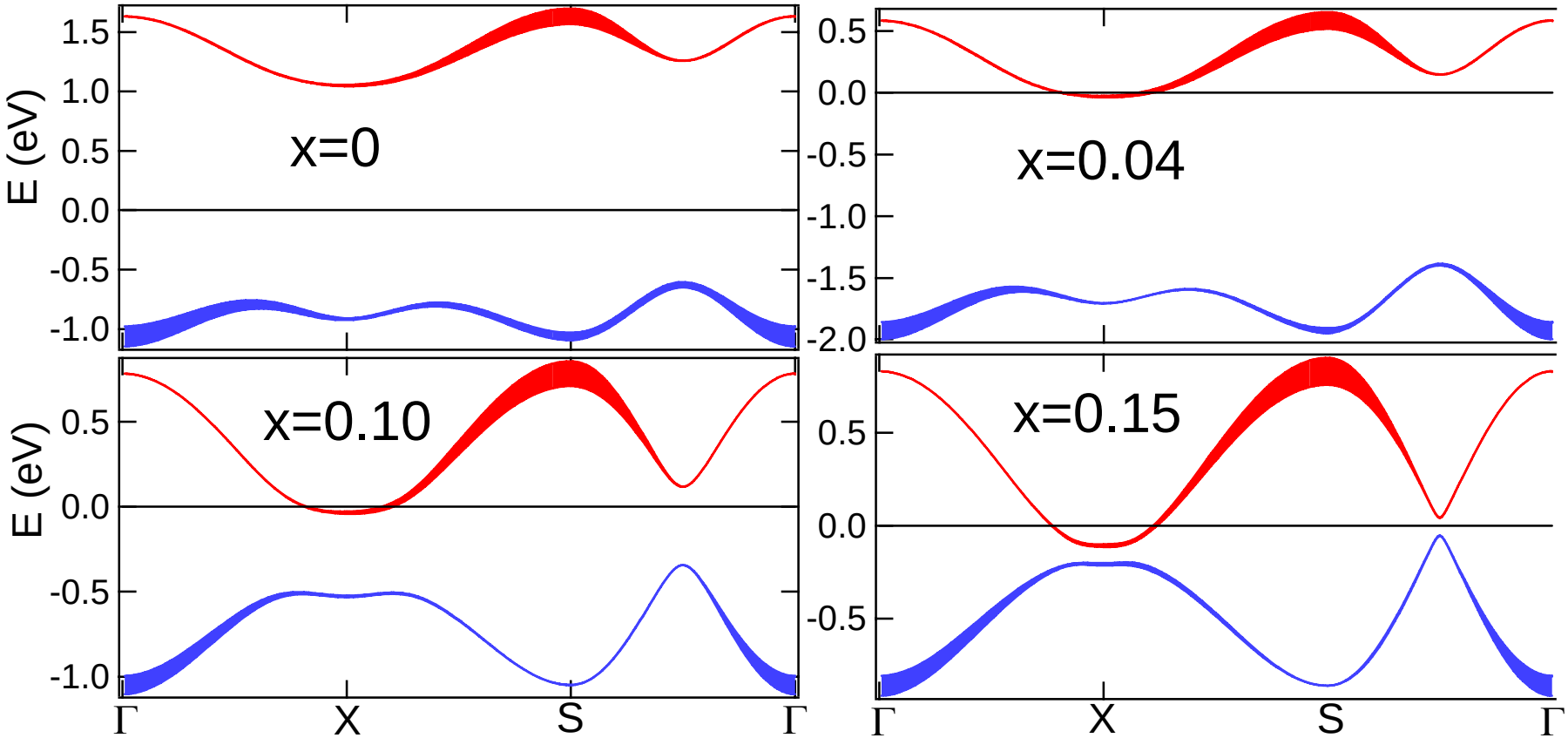

E: Armitage, et al. PRL88, 257001 (02); T: Kusko, et al. PRB66, 140513 (02)

# Collapse of Mott Gap

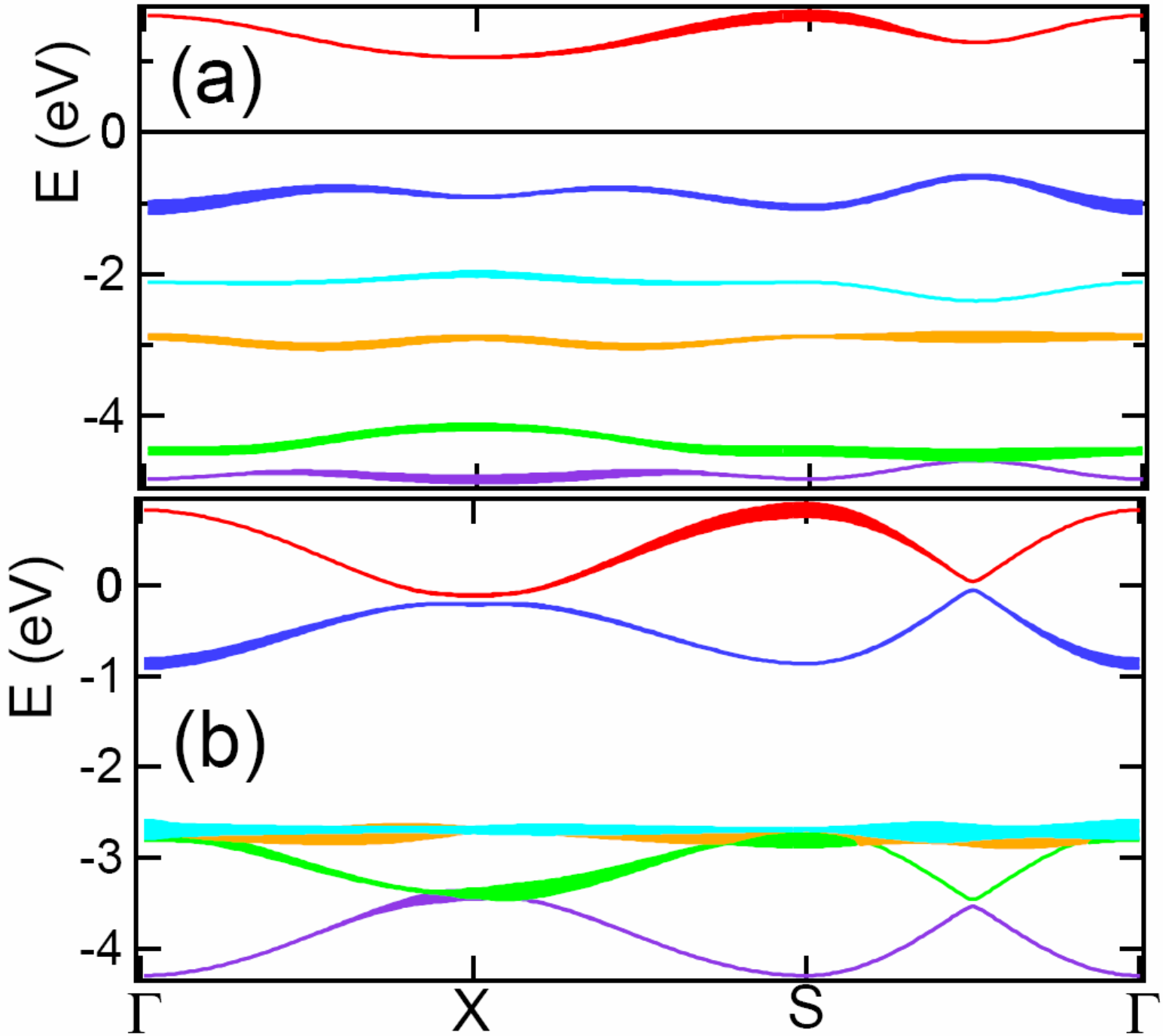



**Mean Field Calculation**

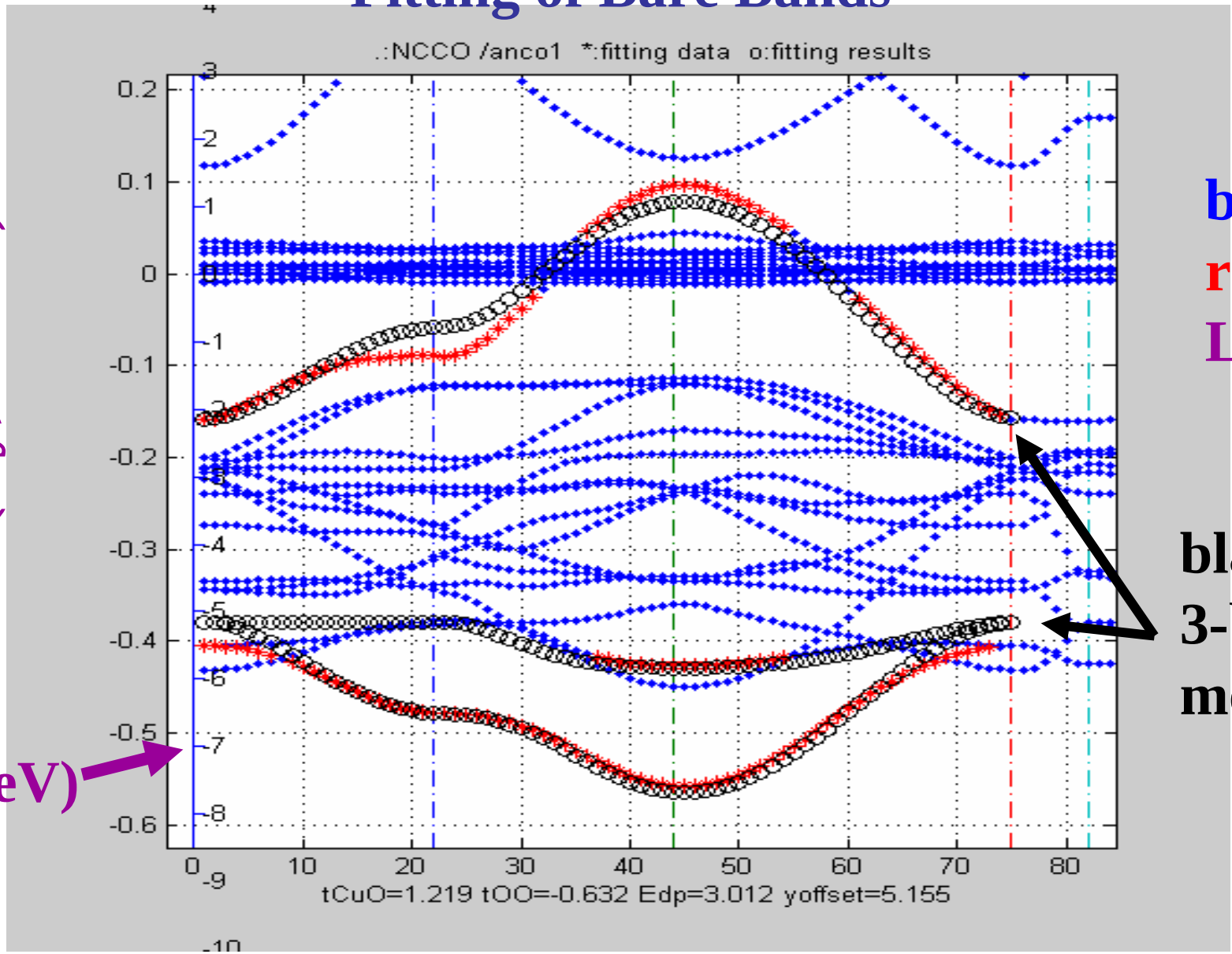
# Three Band Model



$$
\begin{aligned}
H = & \sum_{j} (\Delta_0 d_j^\dagger d_j + U n_{j\uparrow} n_{j\downarrow}) \\
& + \sum_{<i,j>} t_{CuO} [d_j^\dagger p_i + (c.c.)] \\
& + \sum_{<<i,i'>>} t_{OO} [p_i^\dagger p_{i'} + (c.c.)] \\
& + \sum_{i} U_p n_{i\uparrow} n_{i\downarrow}.
\end{aligned}
$$


(a)
E (eV)
0
-2
-4
(b)
E (eV)
0
-1
-2
-3
-4
Γ
X
S
Γ

# Fitting of Bare Bands




E (Ry, or eV)

(eV)

blue, red = LDA

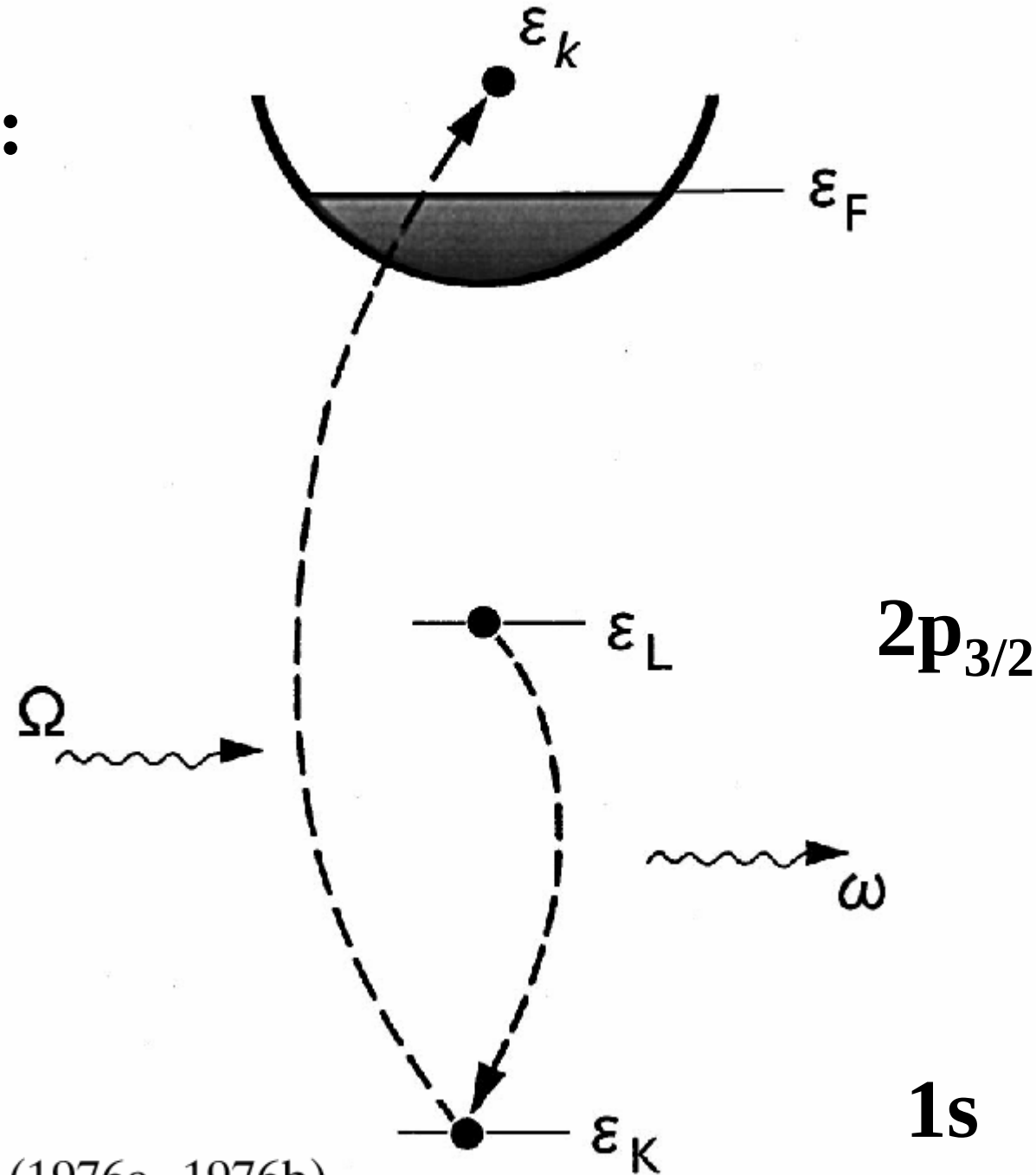
black = 3-band model

Γ (π,0) (π,π) Γ

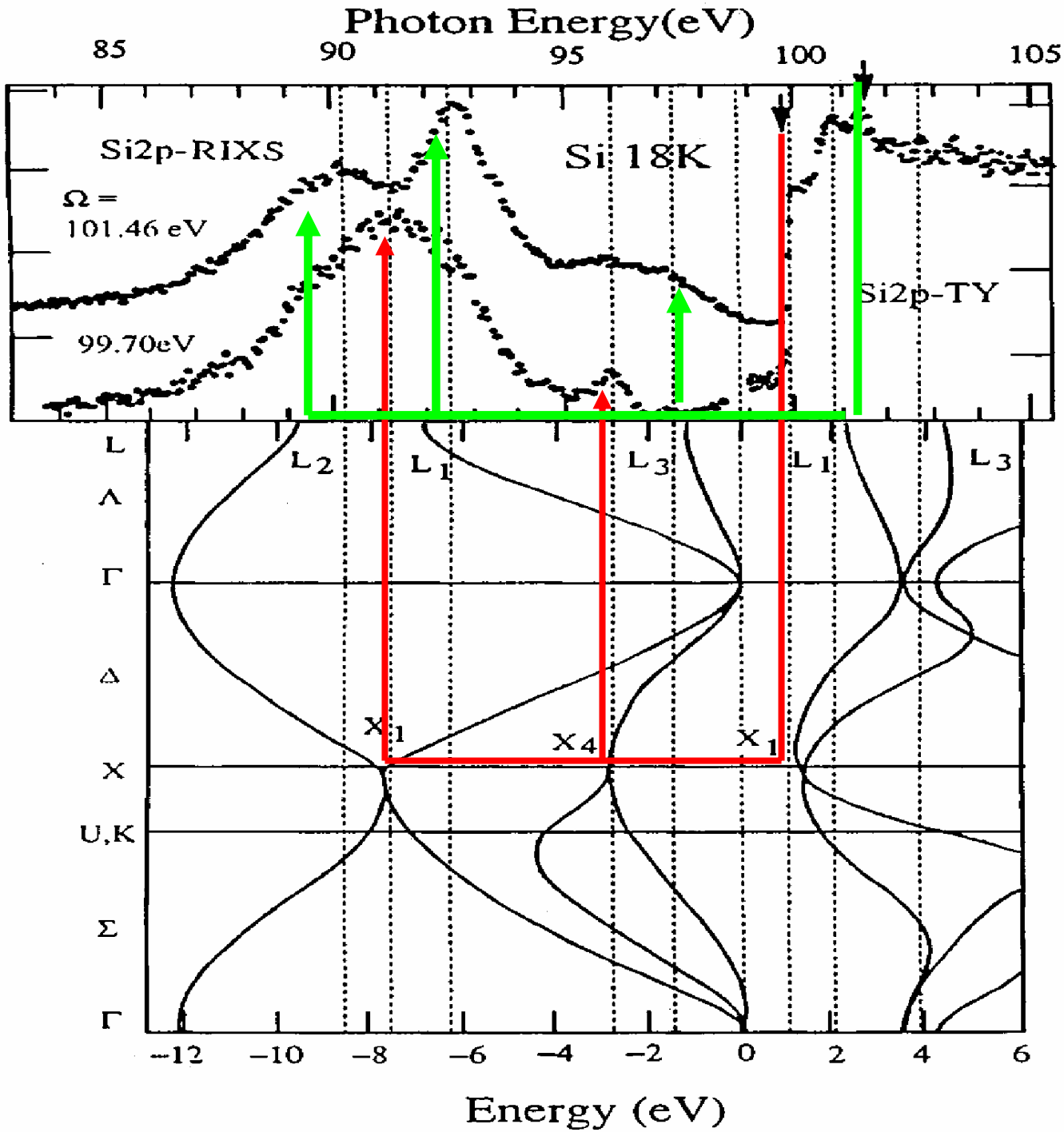
red = $CuO_2$ bands

# Resonant Inelastic X-ray Scattering (RIXS)

# Cu metal:




Eisenberger *et al.* (1976a, 1976b)

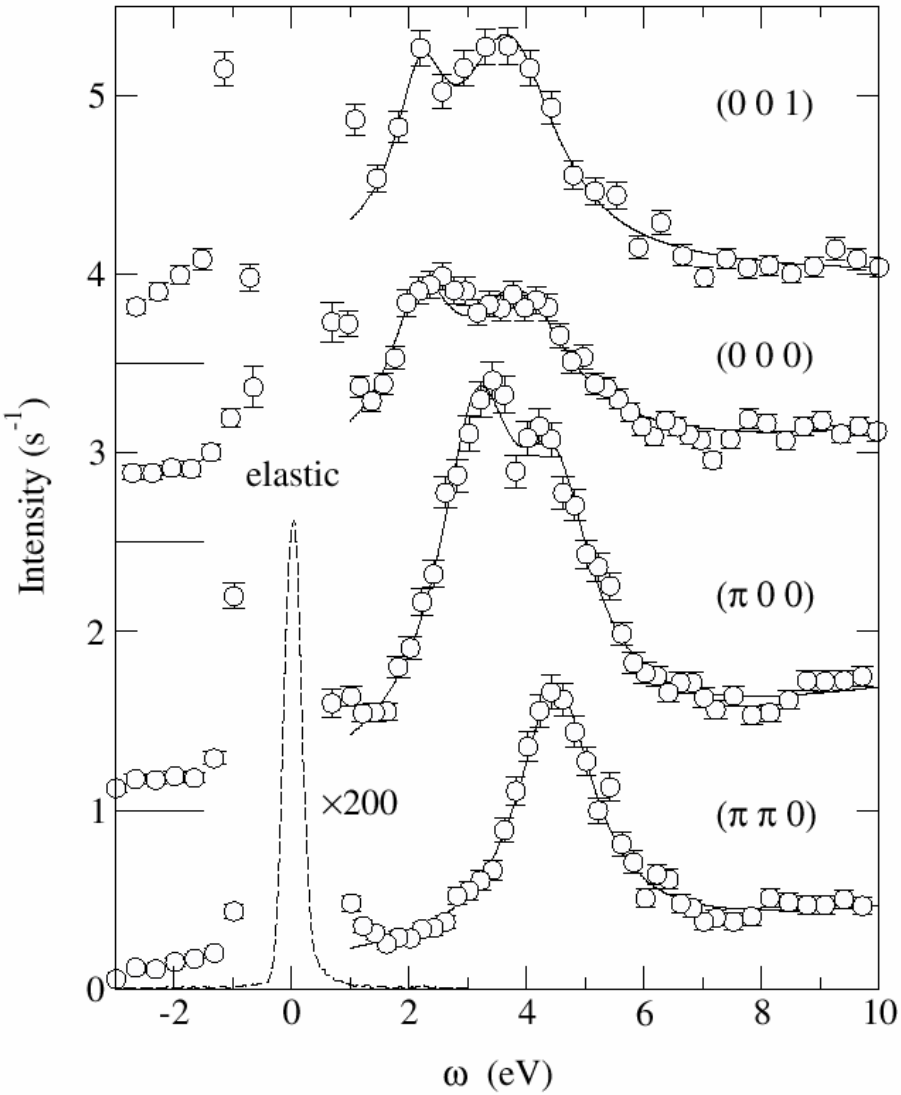

Photon Energy(eV)
85
90
95
100
105
Si2p-RIXS
Ω =
101.46 eV
99.70eV
Si 18K
Si2p-TY
L
Λ
Γ
Δ
X
U,K
Σ
Γ
L2
L1
L3
L1
L3
X1
X4
X1
−12
−10
−8
−6
−4
−2
0
2
4
6
Energy (eV)

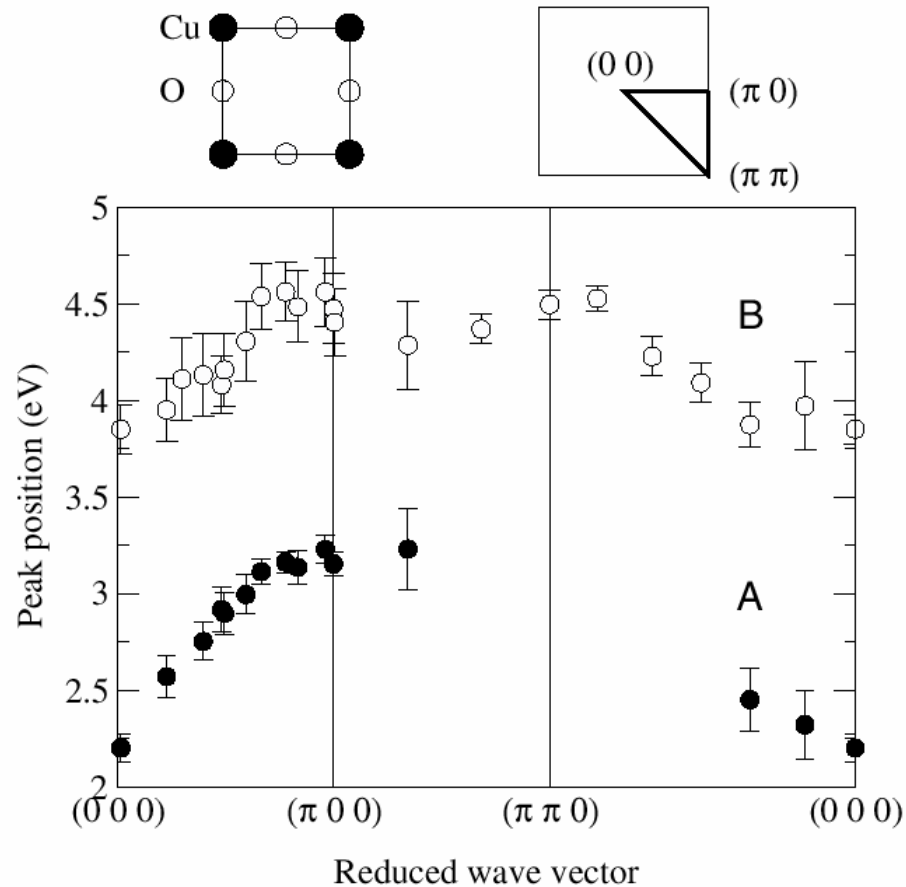
**Si**

# Application to Cuprates

- **R.S. Markiewicz and A. Bansil, cond-mat/0506474**

# $La_2CuO_4$: Kim, et al., PRL89, 177003 (02)



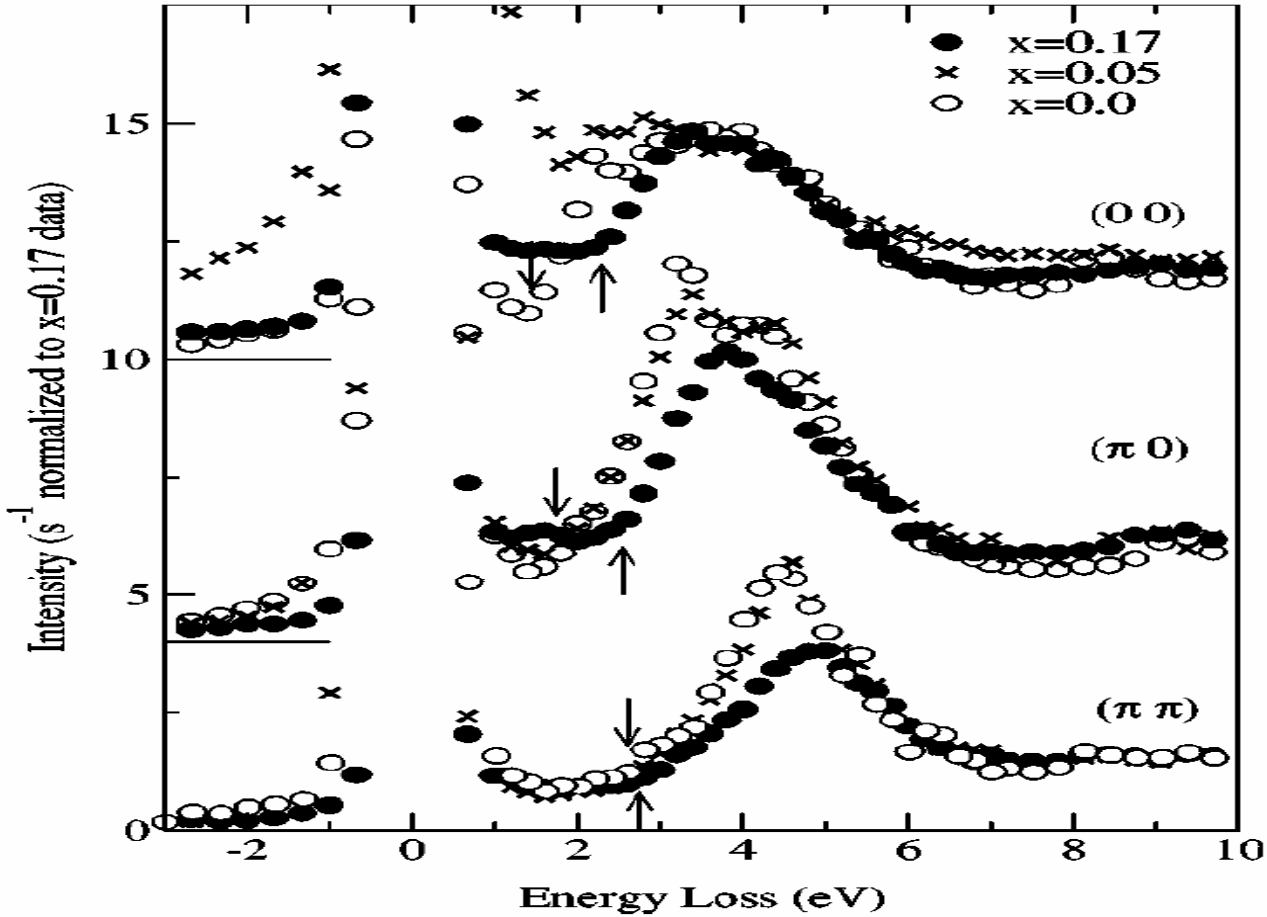
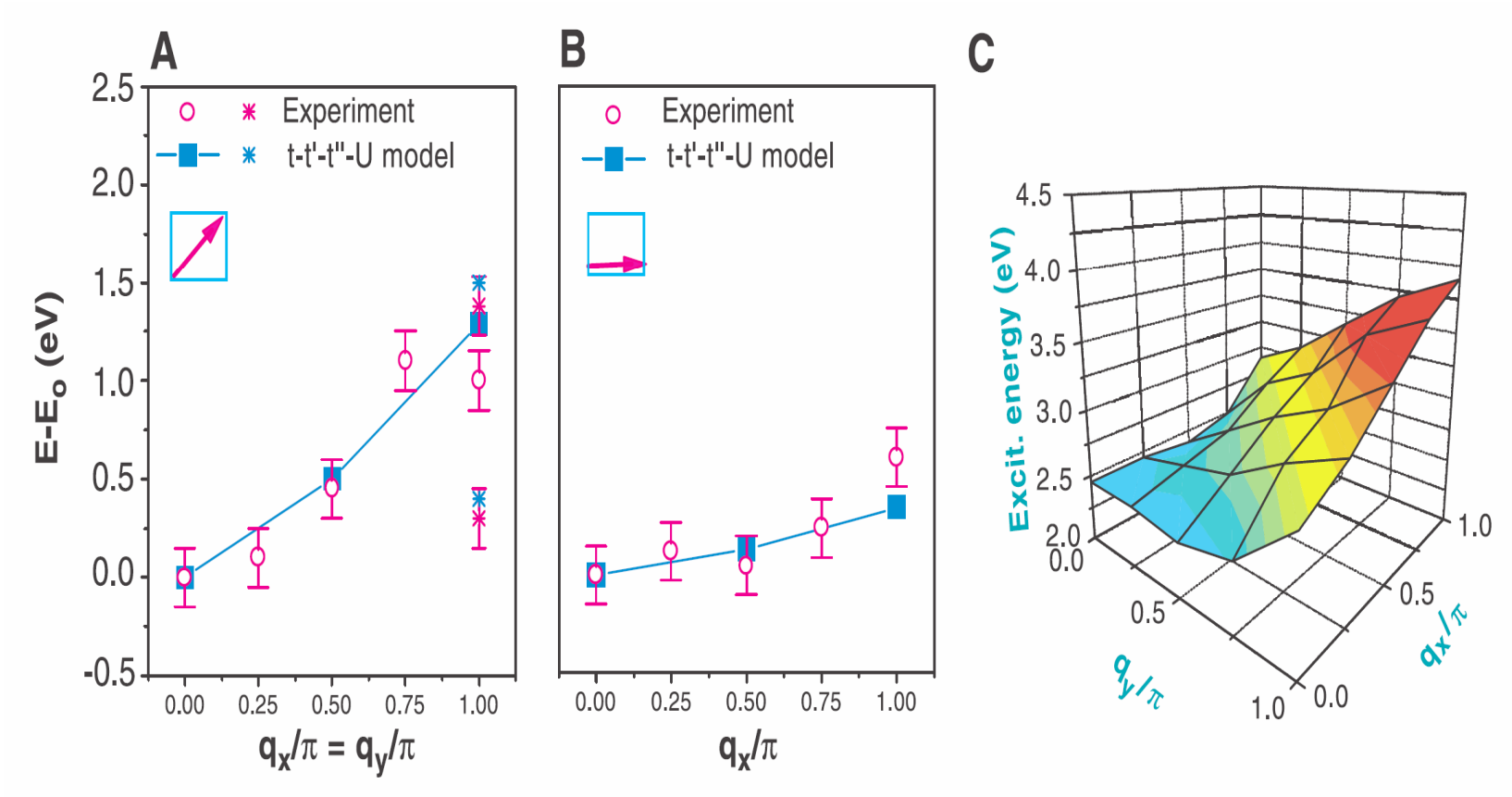



FIG. 5. Comparison of RIXS spectra at selected momenta for the $x=0$, $x=0.05$, and $x=0.17$ samples of $La_{2-x}Sr_xCuO_4$. The (0 0) and ($\pi$ 0) data are shifted for clarity. The up and down arrows denote the onset energy of the spectra for the $x=0.17$ and $x=0$ samples, respectively.

Y.-J. Kim, J. P. Hill, S. Komiya, Y. Ando, D. Casa, T. Gog, and C. T. Venkataraman Phys. Rev. B **70,** 094524 (2004)**.**

# NCCO




**Hasan, et al., Science 288, 1811 (2000)**

$$W(\mathbf{q},\omega,\omega_i) = (2\pi)^3 N |w(\omega,\omega_i)|^2$$

$$\times \sum_{\mathbf{k}jj'} \delta(\omega + E_j(\mathbf{k}) - E_{j'}(\mathbf{k}+\mathbf{q})) n_j(\mathbf{k})[1 - n_{j'}(\mathbf{k}+\mathbf{q})]$$

$$\times \Big| \sum_{\ell,\sigma,\sigma'} e^{i\mathbf{q}\cdot\mathbf{R}_\ell} \alpha_\ell X^j_{\ell\sigma} \Lambda_{\sigma,\sigma'}(\omega,\mathbf{q}) X^{j'}_{\ell\sigma'} \Big|^2,$$

**AF coherence factor**

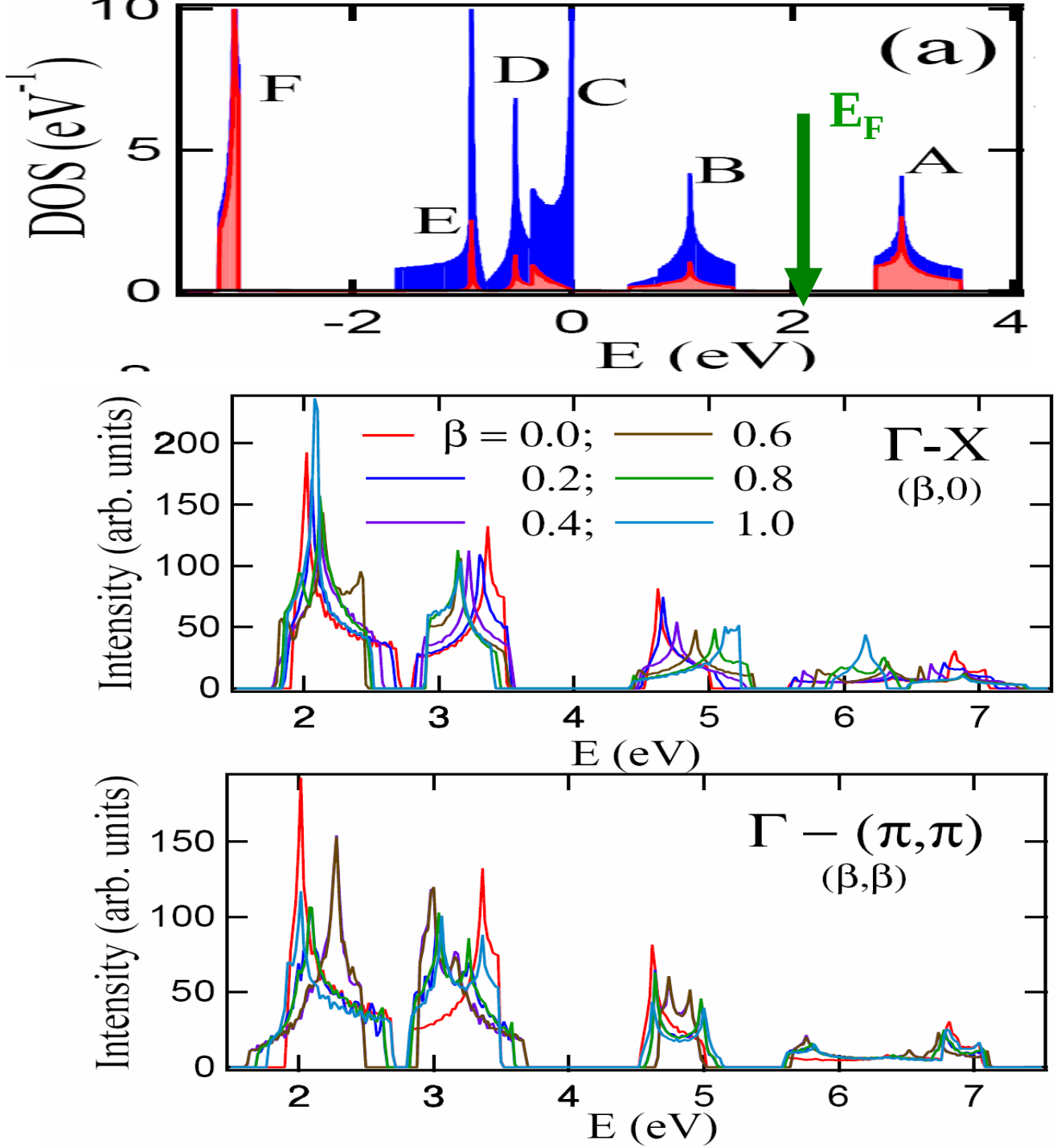
**Cu vs O weight**

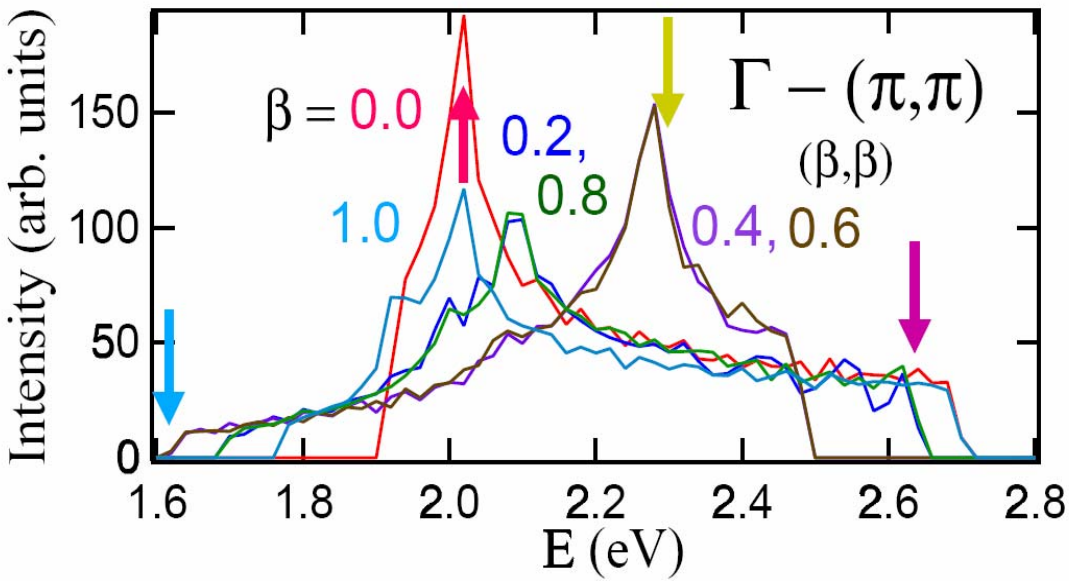
where

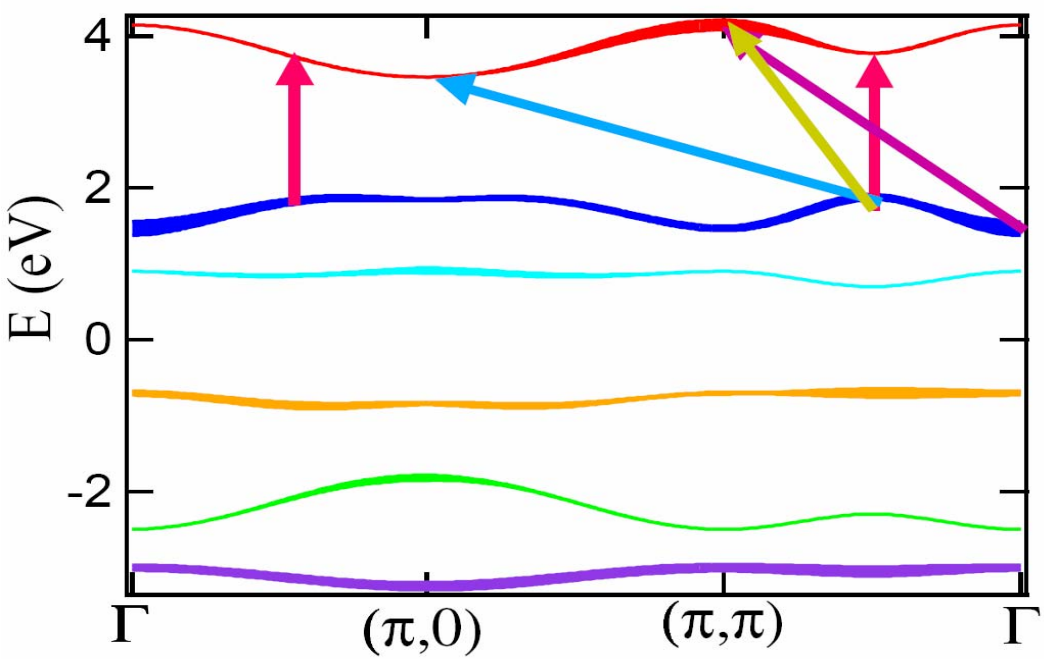
$$w(\omega,\omega_i) = |\gamma|^2 \sum_{\mathbf{k_1}} \frac{V_d}{D(\omega_i,\mathbf{k_1}) D(\omega_f,\mathbf{k_1})}.$$

$$D_j = \omega_j + \epsilon_{1s} - \epsilon_{4p}(\mathbf{k_1}) + i\Gamma_{1s},\ j = i, f.$$

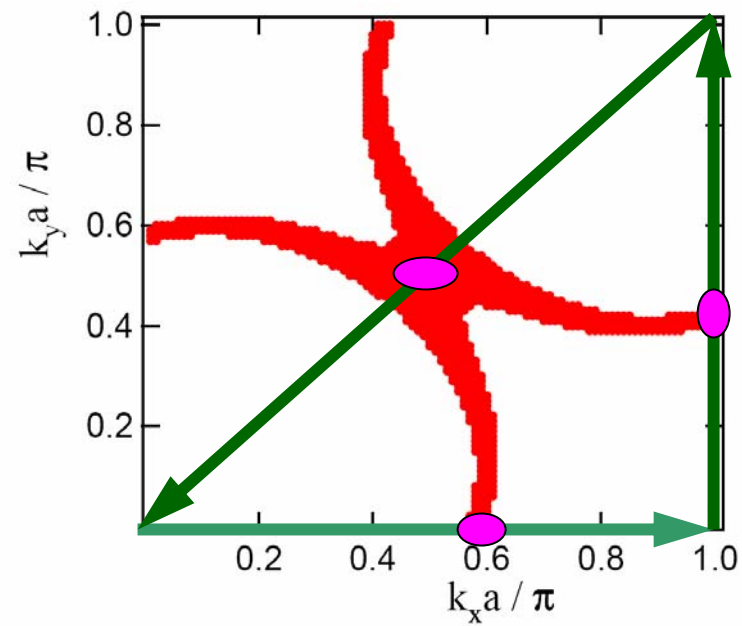
$$\Lambda_{\sigma,\sigma'} = \delta_{\sigma,\sigma'}$$


(a)
DOS (eV$^{-1}$)
F
E
D
C
B
A
$E_F$
E (eV)
β = 0.0; 0.2; 0.4; 0.6 0.8 1.0
Γ-X
(β,0)
Intensity (arb. units)
E (eV)
Γ − (π,π)
(β,β)
Intensity (arb. units)
E (eV)

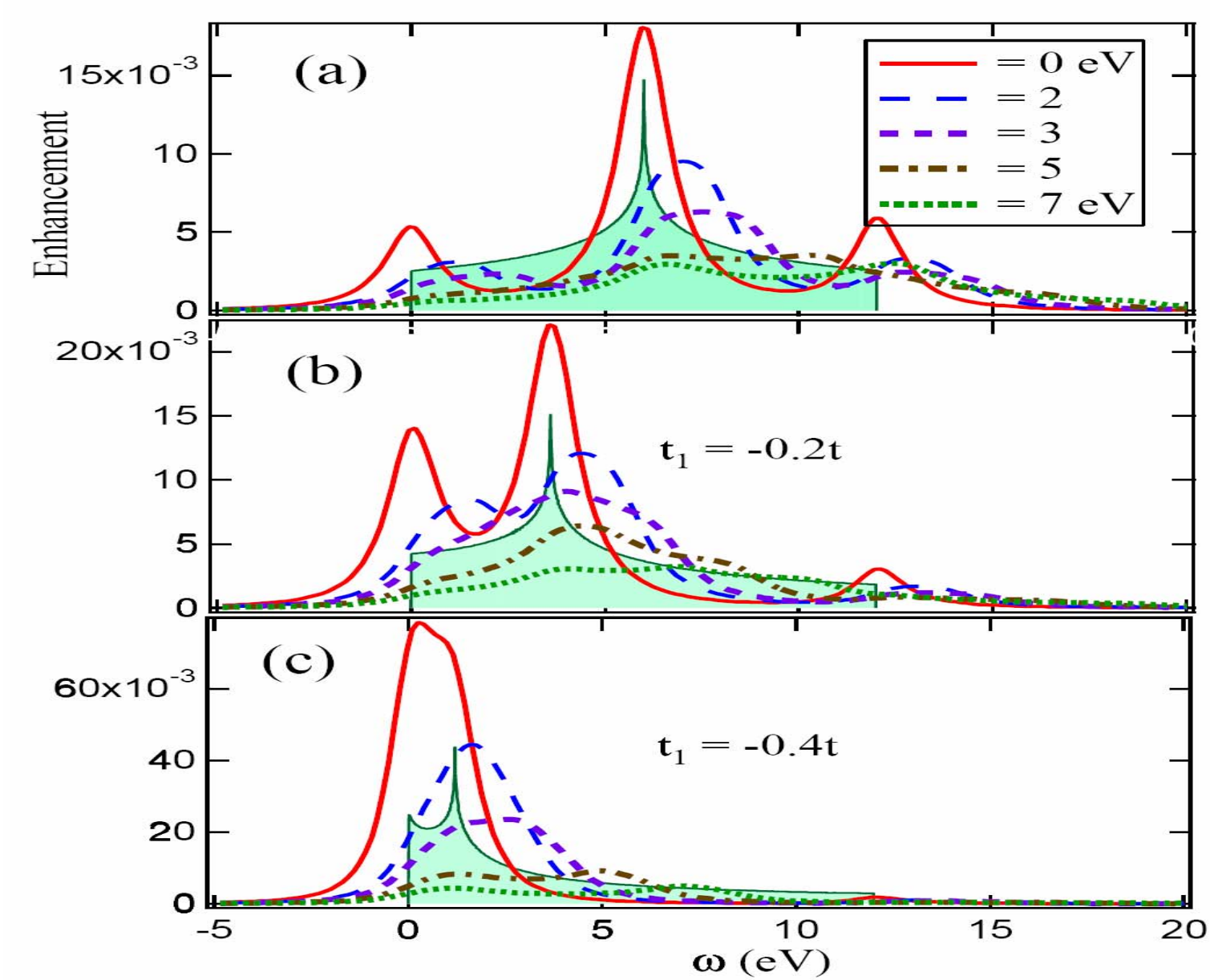

Intensity (arb. units)
150
100
50
0
1.6
1.8
2.0
2.2
2.4
2.6
2.8
E (eV)
β = 0.0
0.2,
0.8
1.0
0.4, 0.6
Γ – (π,π)
(β,β)

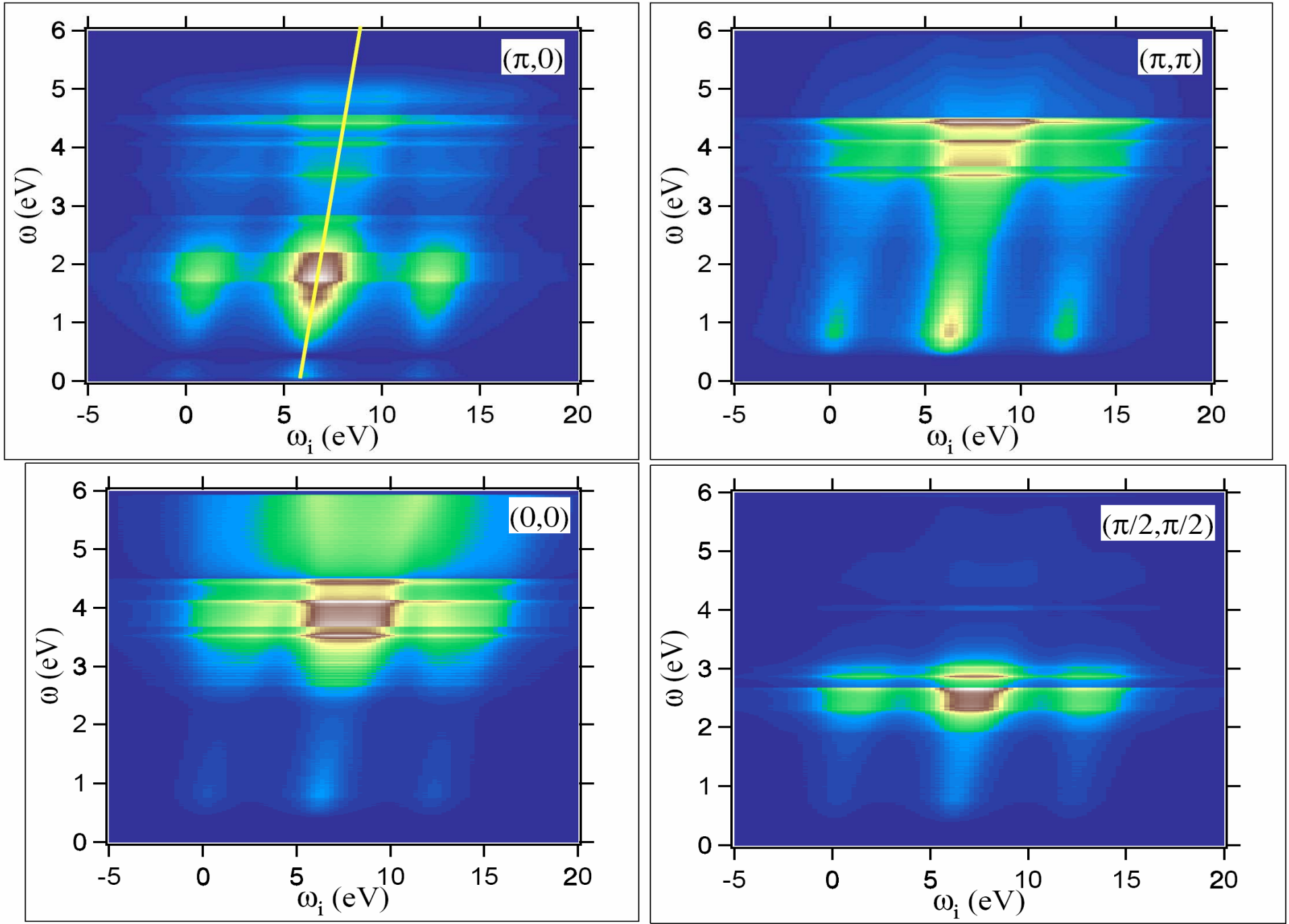

E (eV)
4
2
0
-2
Γ
(π,0)
(π,π)
Γ

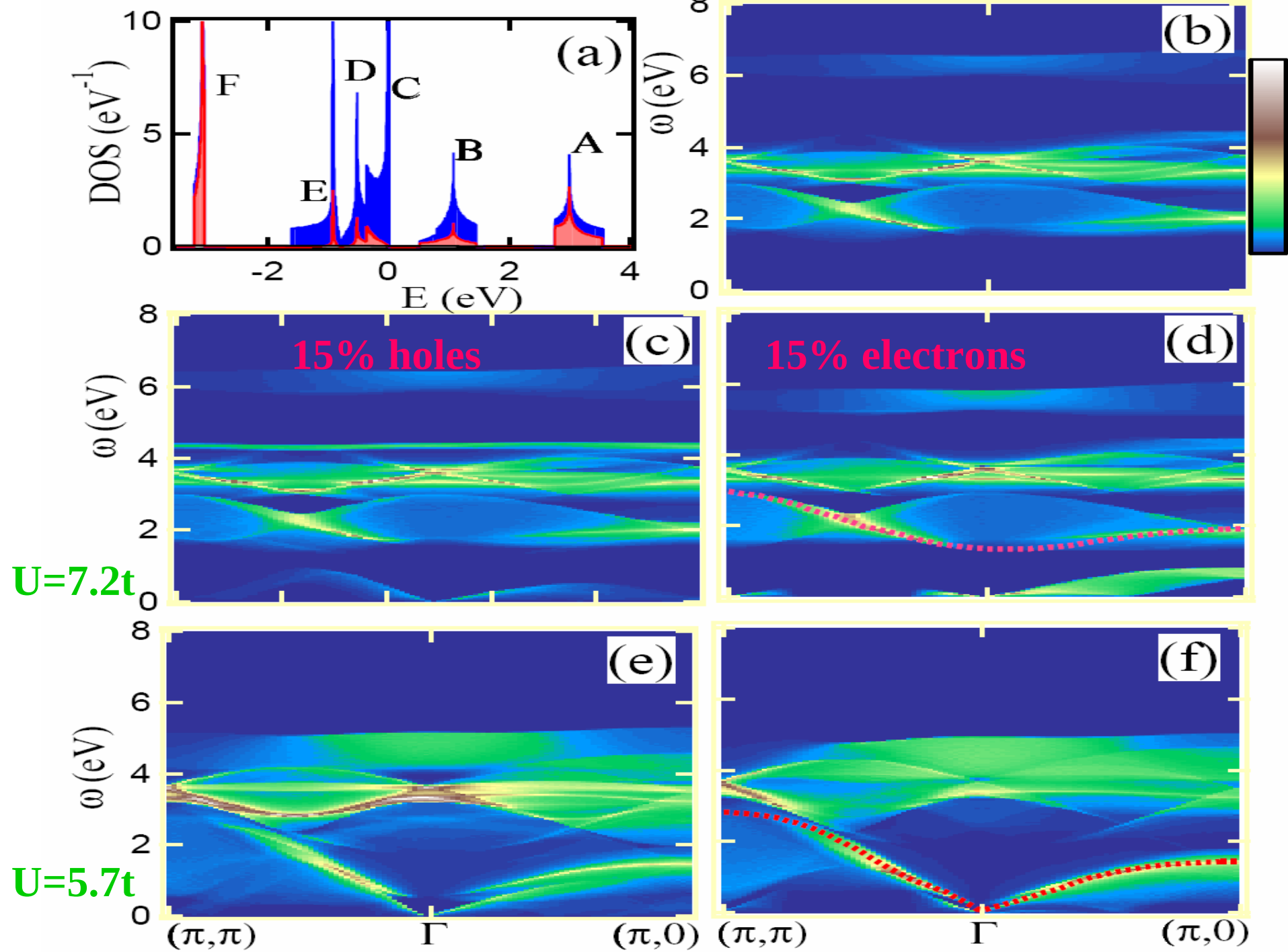
Γ:

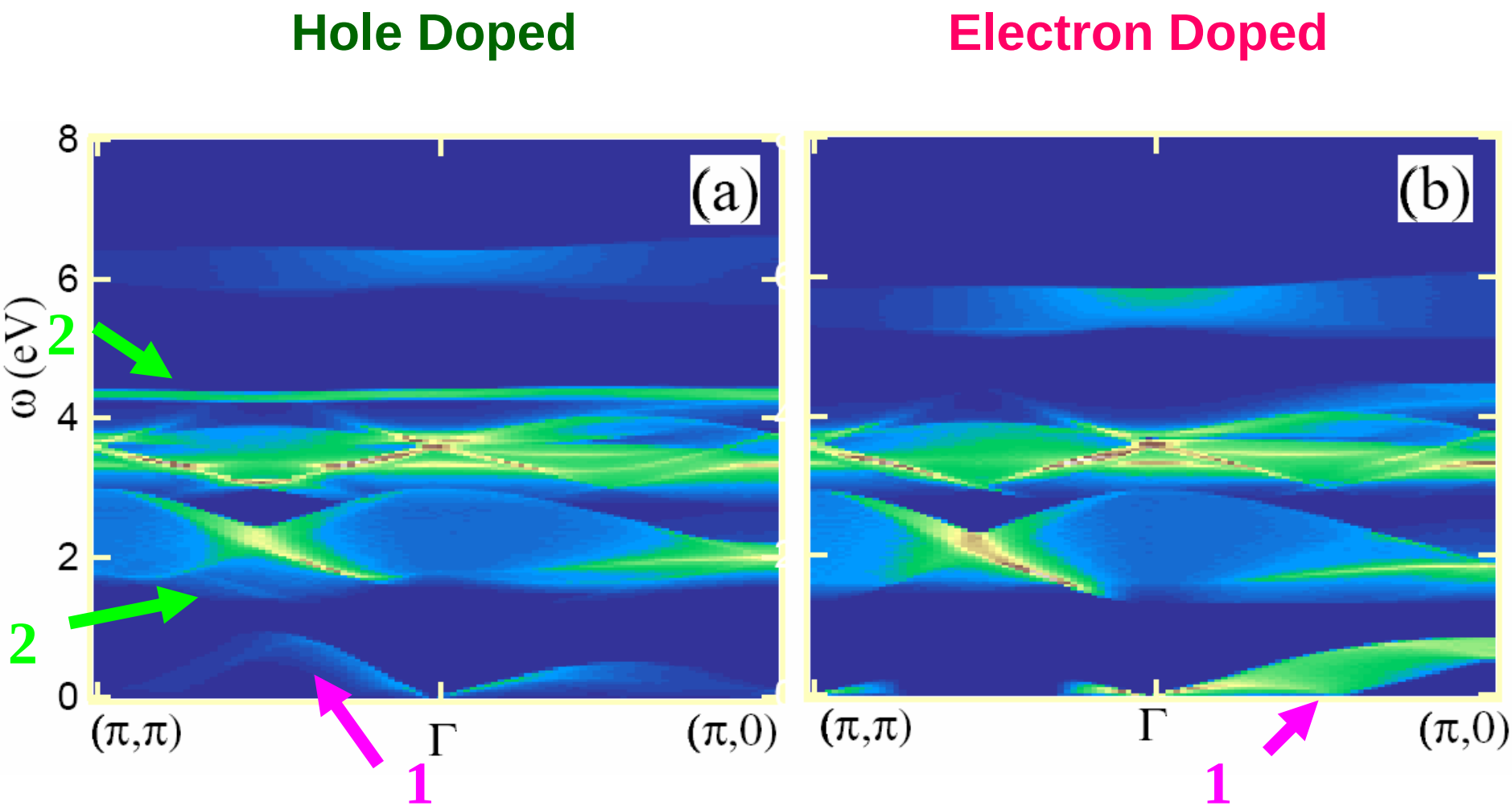

1.0
0.8
0.6
0.4
0.2
$k_y a / \pi$
0.2
0.4
0.6
0.8
1.0
$k_x a / \pi$

# Resonance Factor

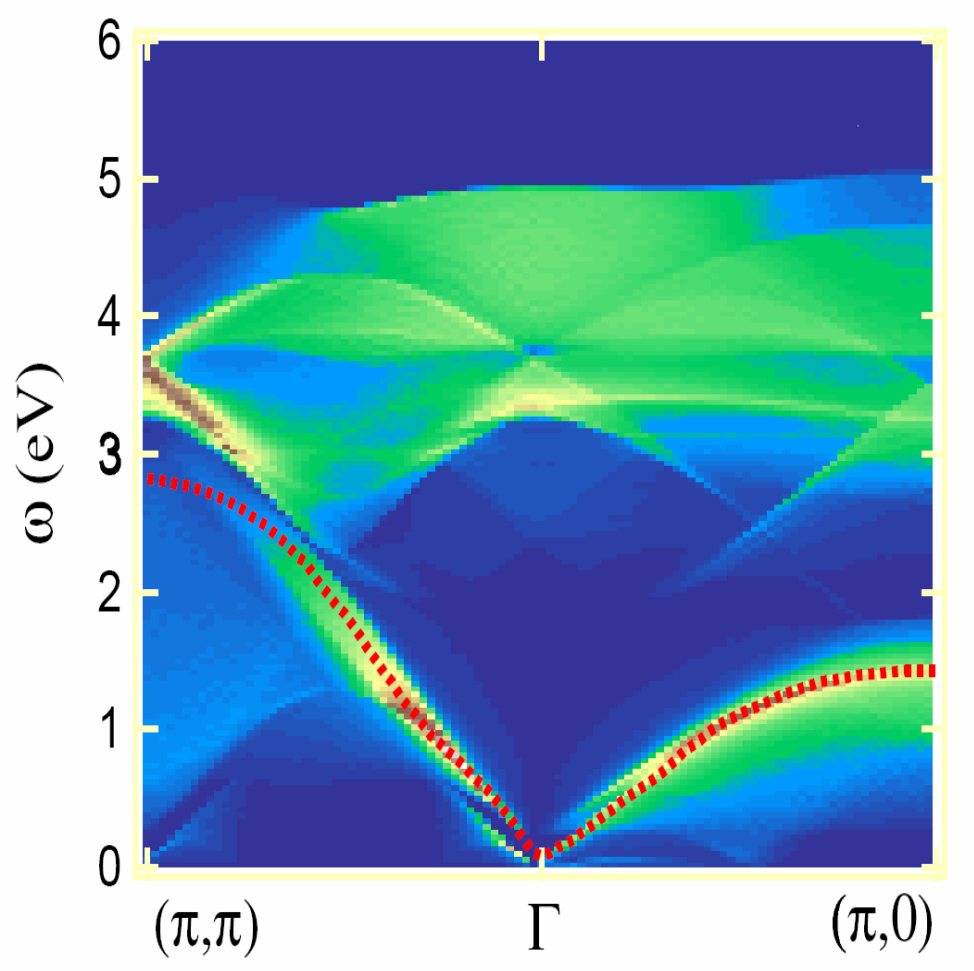



(π,0)
(π,π)
(0,0)
(π/2,π/2)
ω (eV)
ω_i (eV)
-5
0
5
10
15
20
0
1
2
3
4
5
6


(a)
DOS (eV$^{-1}$)
E (eV)
F
E
D
C
B
A
(b)
(c)
15% holes
(d)
15% electrons
(e)
(f)
ω (eV)
U=7.2t
U=5.7t
(π,π)
Γ
(π,0)

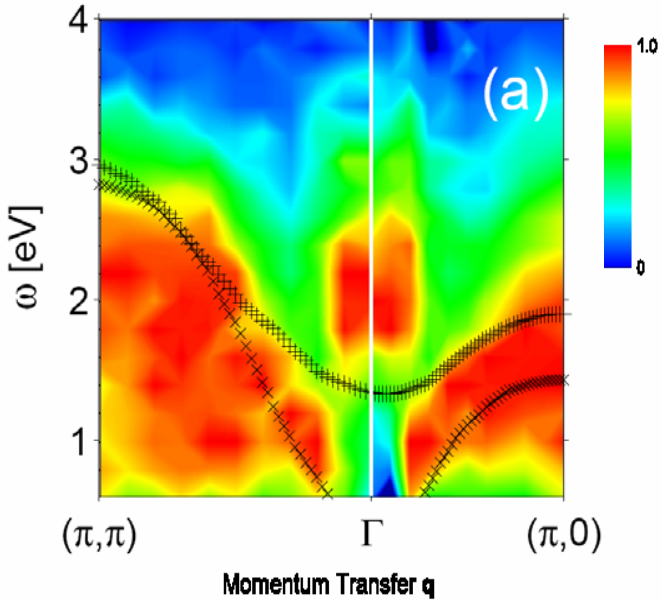

Hole Doped
Electron Doped
(a)
(b)
ω (eV)
8
6
4
2
0
2
2
1
1
(π,π)
Γ
(π,0)
(π,π)
Γ
(π,0)

# Electron Doped



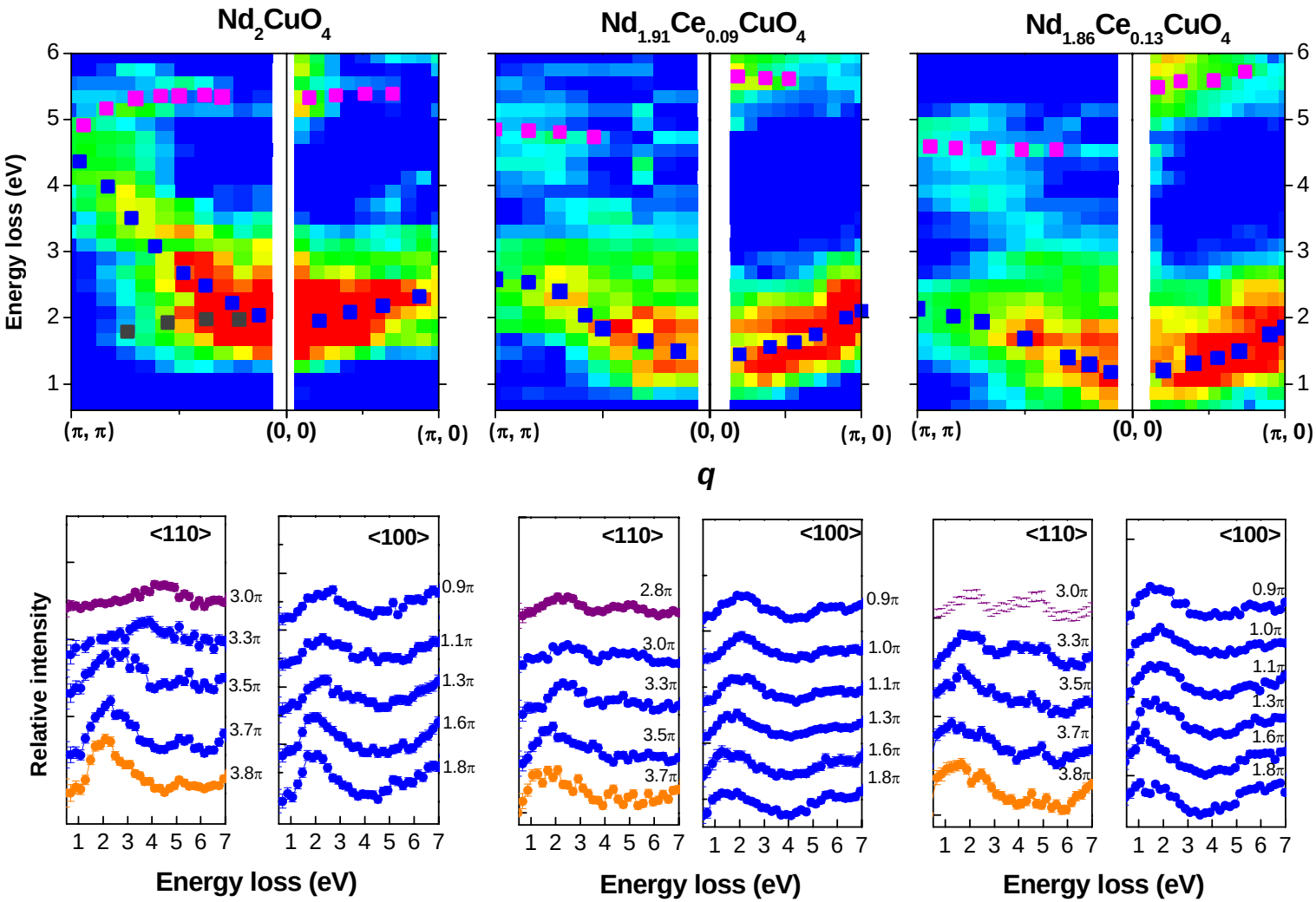

**x=-0.15**

**NCCO, x=-0.15**

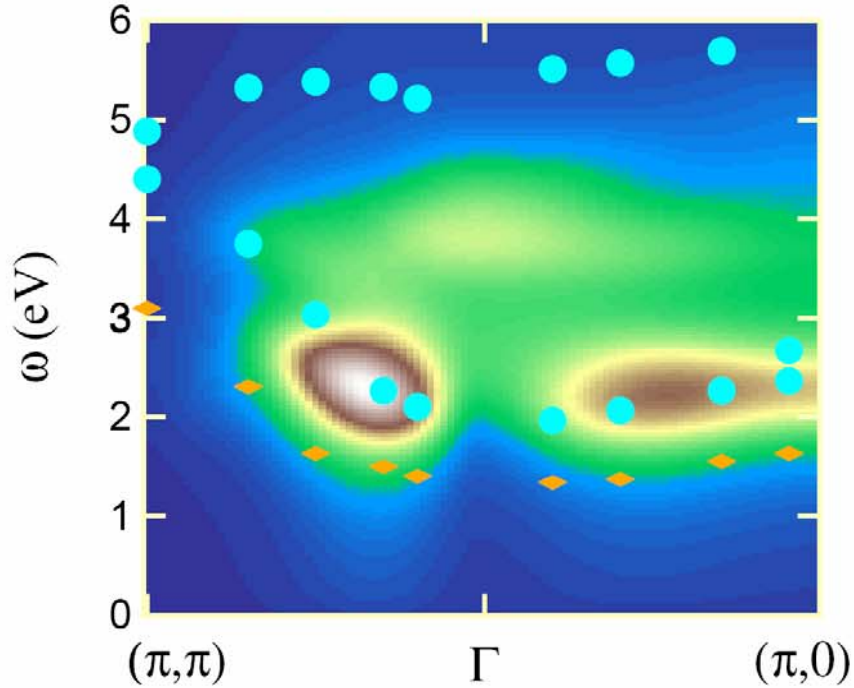


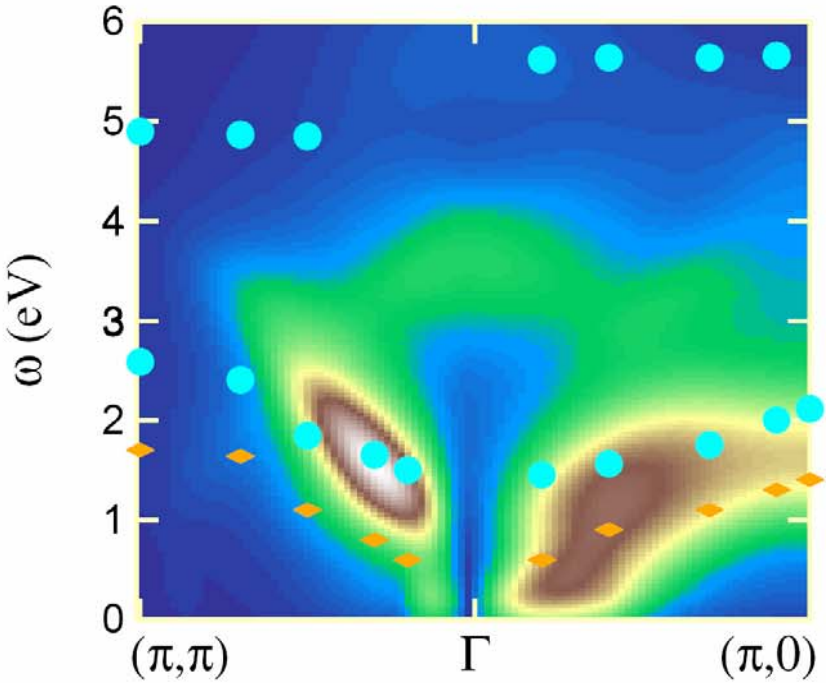

Ishii, *et al.* c-m/0412467

# Doping Evolution of Particle-hole Modes in electron-doped Cuprates



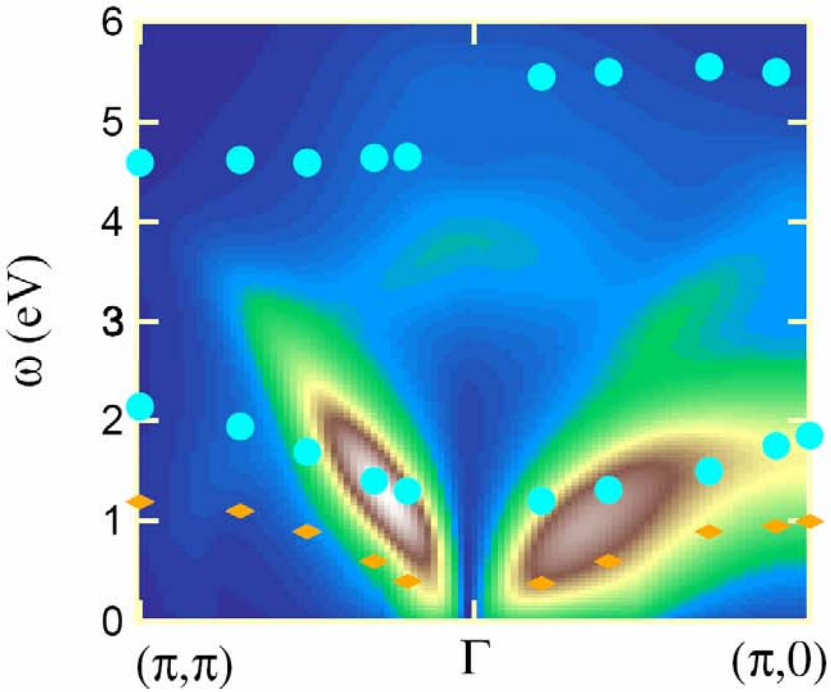

Li, Qian, Hasan et.al., (Princeton University)




***x=0.00***

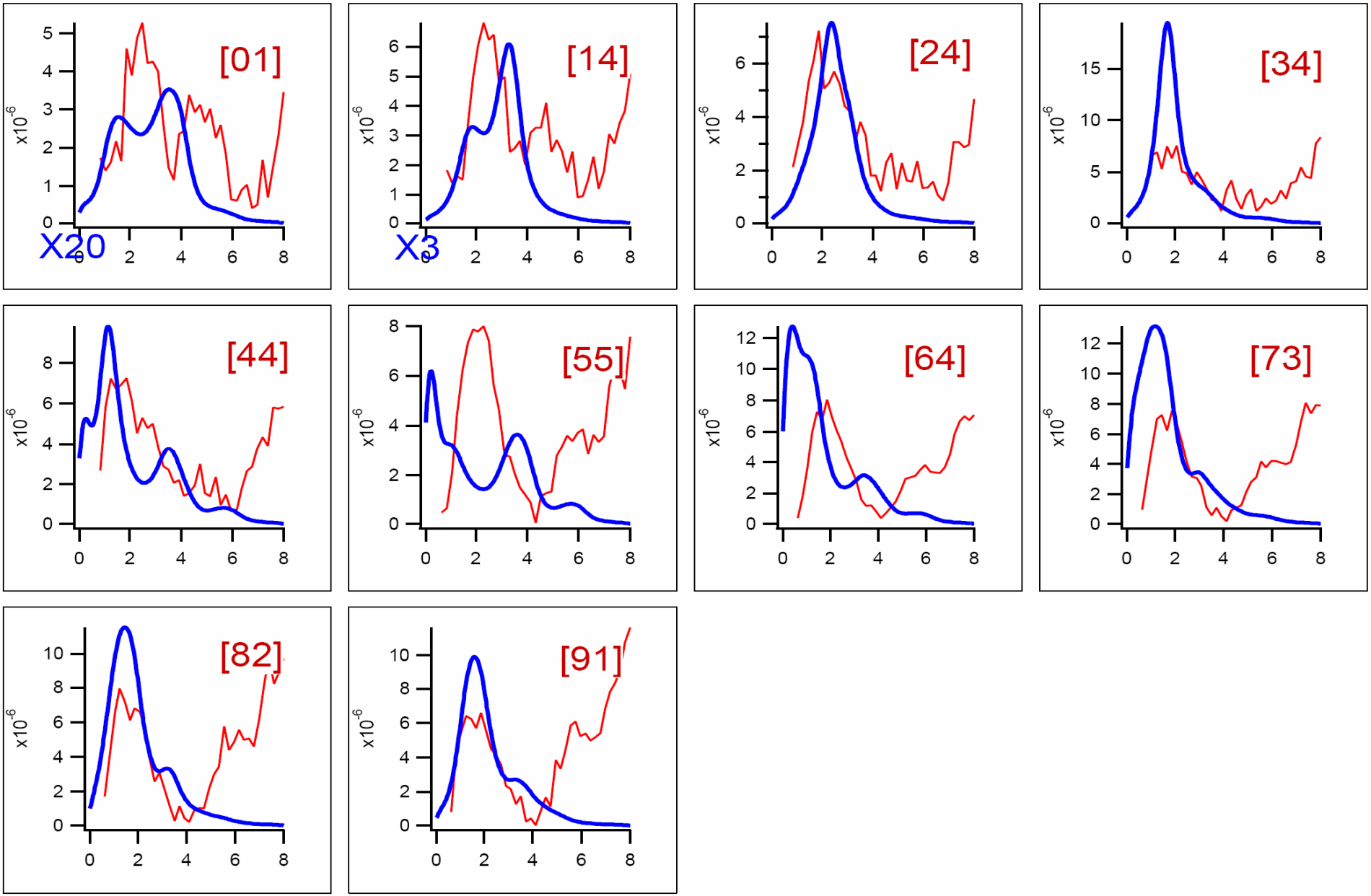
***x=0.09***

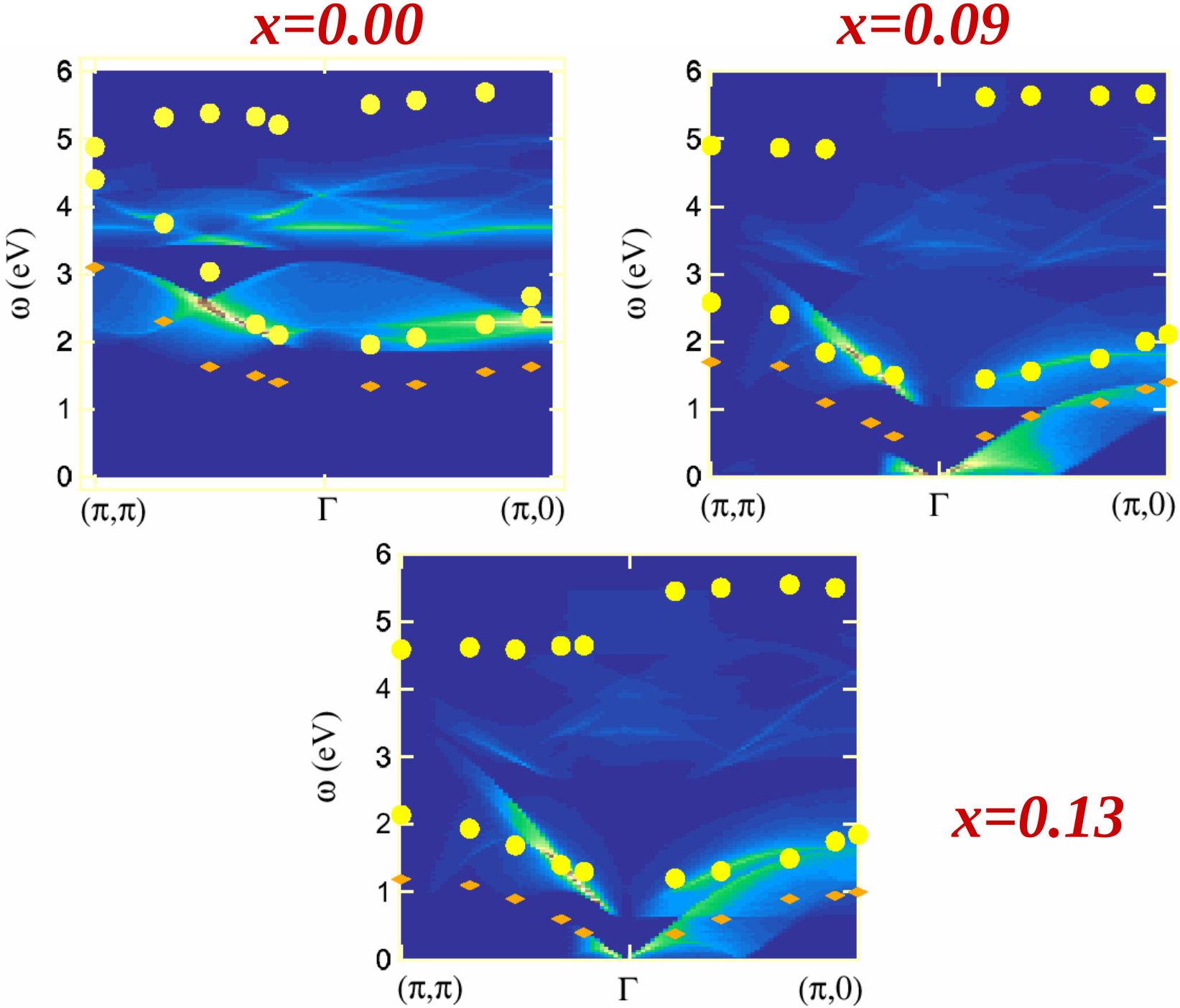



**Σ''=300meV**

***x=0.13***

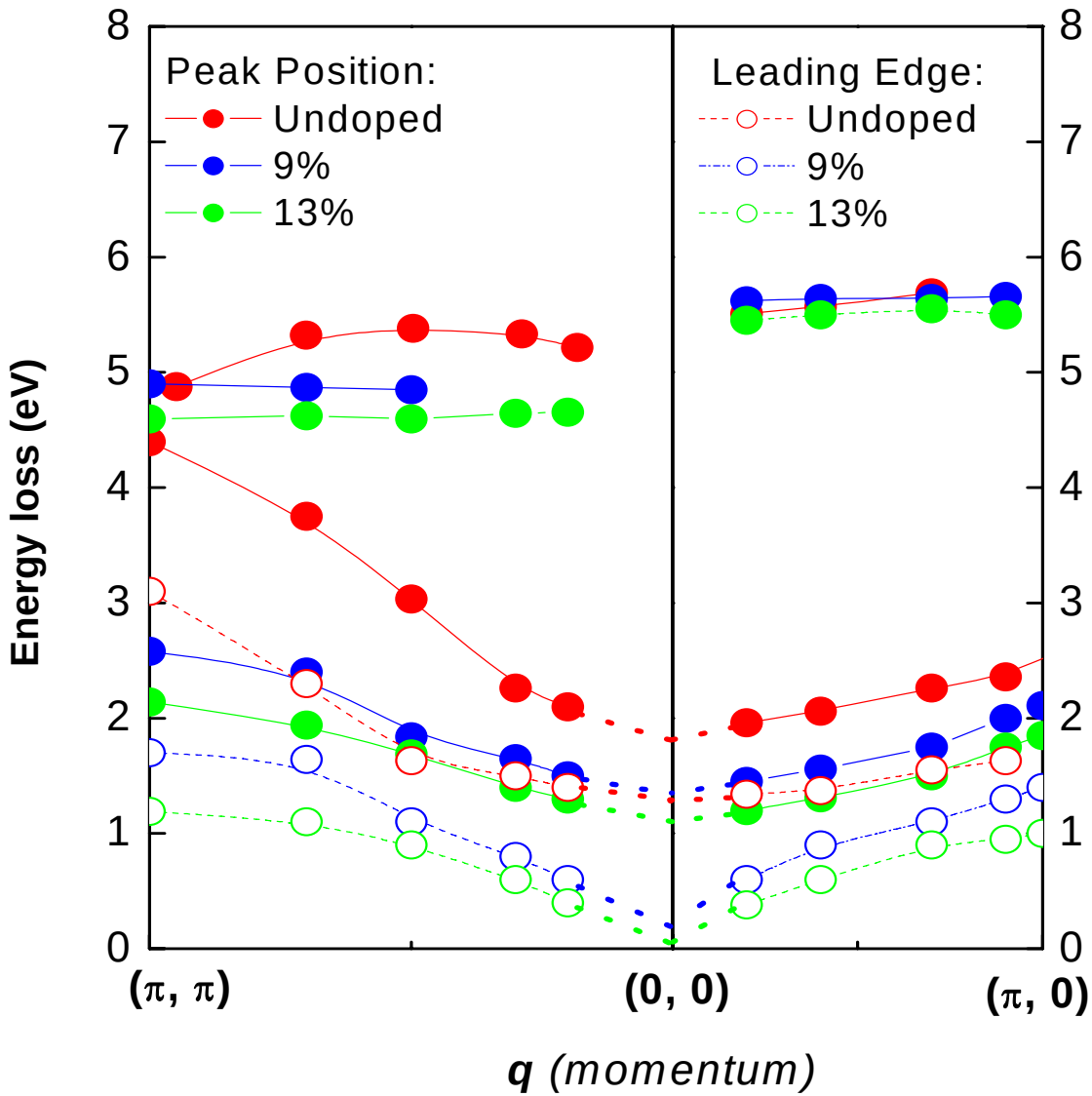
# $x=0.09$

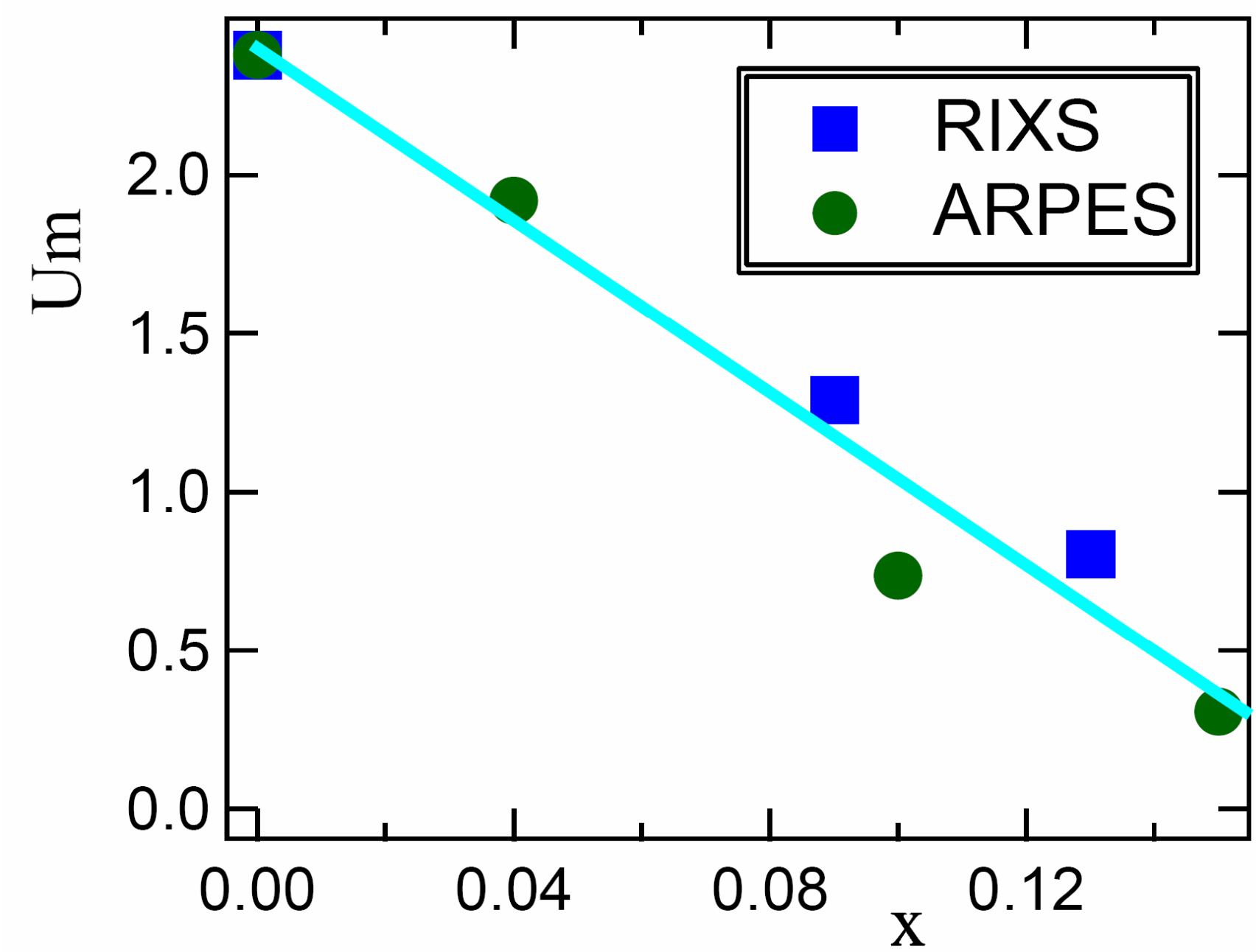



x=0.00
x=0.09
x=0.13
ω (eV)
0
1
2
3
4
5
6
(π,π)
Γ
(π,0)

# Observation of Systematic Gap collapse in doped NCCO

Li, Qian, Hasan et.al., 2005 (Princeton Univ.)




RIXS
ARPES
Um
2.0
1.5
1.0
0.5
0.0
0.00
0.04
0.08
0.12
x

# Conclusions

- **NCCO: Mott gap collapse explains:**
  - **ARPES**
  - **Magnetic & Optical Properties**
  - **RIXS**
- **Hole-doped may be more complex (stripes)**