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INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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H4.SMR/1001-12

*IX TRIESTE WORKSHOP ON
OPEN PROBLEMS IN
STRONGLY CORRELATED SYSTEMS*

14 - 25 July 1997

RECENT PHOTOEMISSION DATA FROM HIGH-Tc SUPERCONDUCTORS

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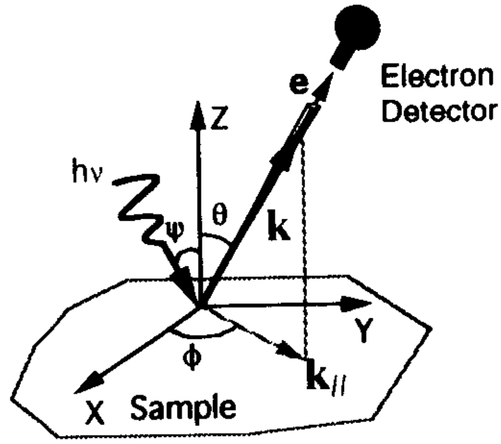
These are preliminary lecture notes, intended only for distribution to participants.

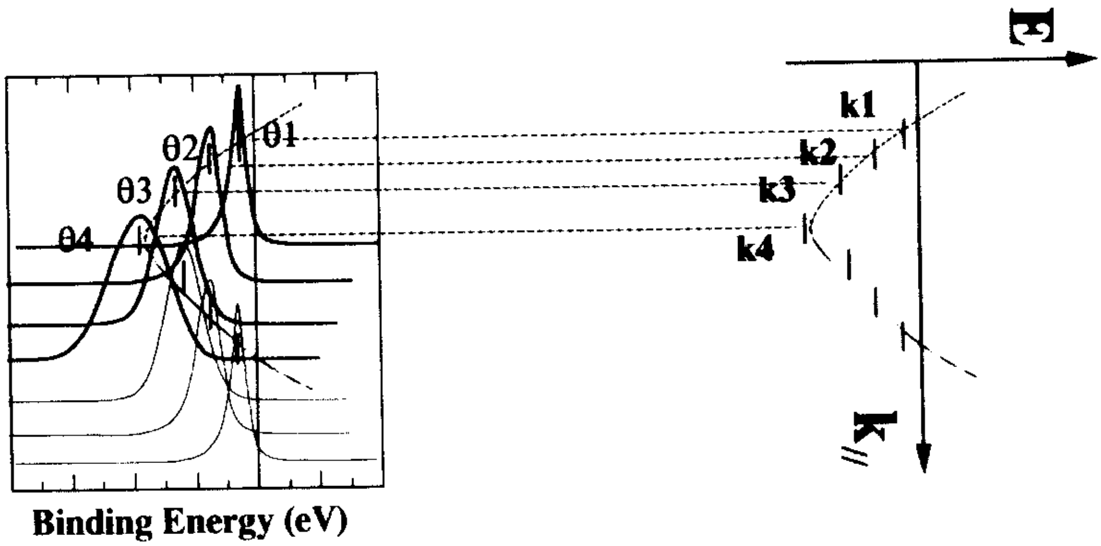
MAIN BUILDING STRADA COSTIERA, 11 TEL. 2240111 TELEFAX 224163 TELEX 460392 ADRIATICO GUEST HOUSE VIA GRIGNANO, 9 TEL.224241 TELEFAX 224531 TELEX 460449
MICROPROCESSOR LAB. VIA BEIRUT, 31 TEL. 2249911 TELEFAX 224600 TELEX 460392 GALILEO GUEST HOUSE VIA BEIRUT, 7 TEL.2240311 TELEFAX 2240310 TELEX 460392
ENRICO FERMI BUILDING VIA BEIRUT, 6 (TELEPHONE, FAX AND TELEX THROUGH MAIN BUILDING)

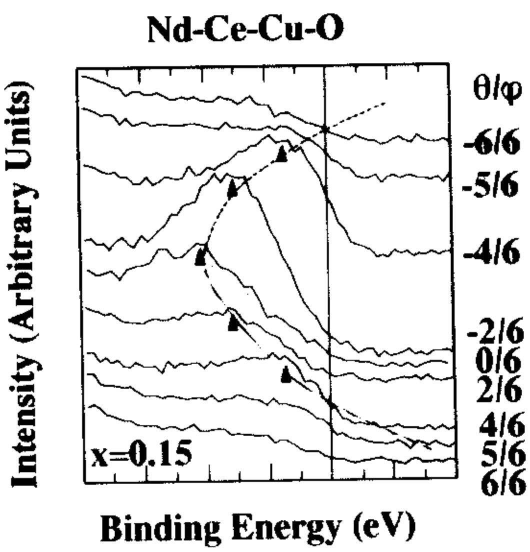
Angle Resolved Photoemission

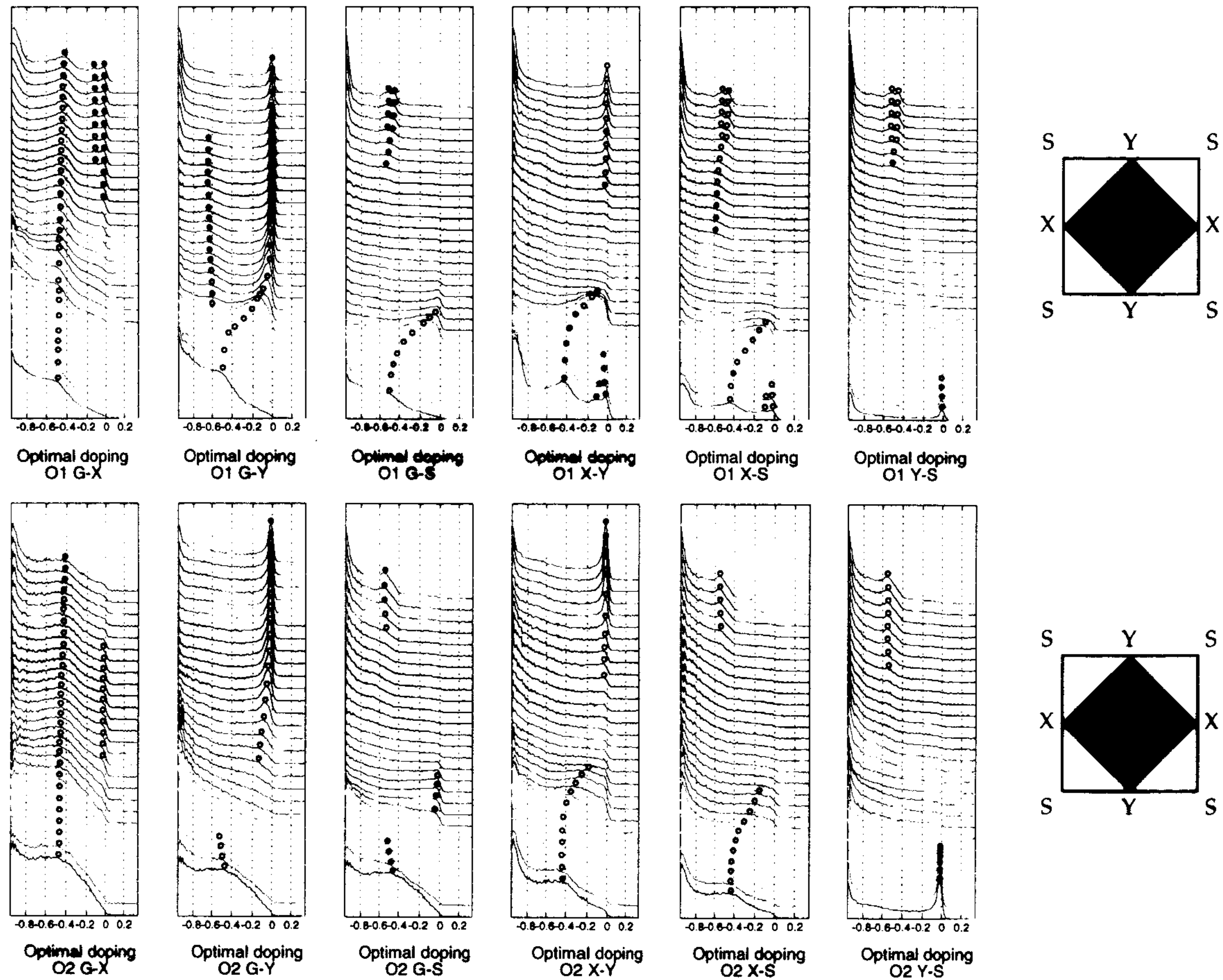
$$\mathbf{k}_{//} = |\mathbf{k}|\mathrm{Sin}\theta$$

$$\mathrm{k} = \sqrt{2\mathrm{E}_{\mathrm{k}}}$$

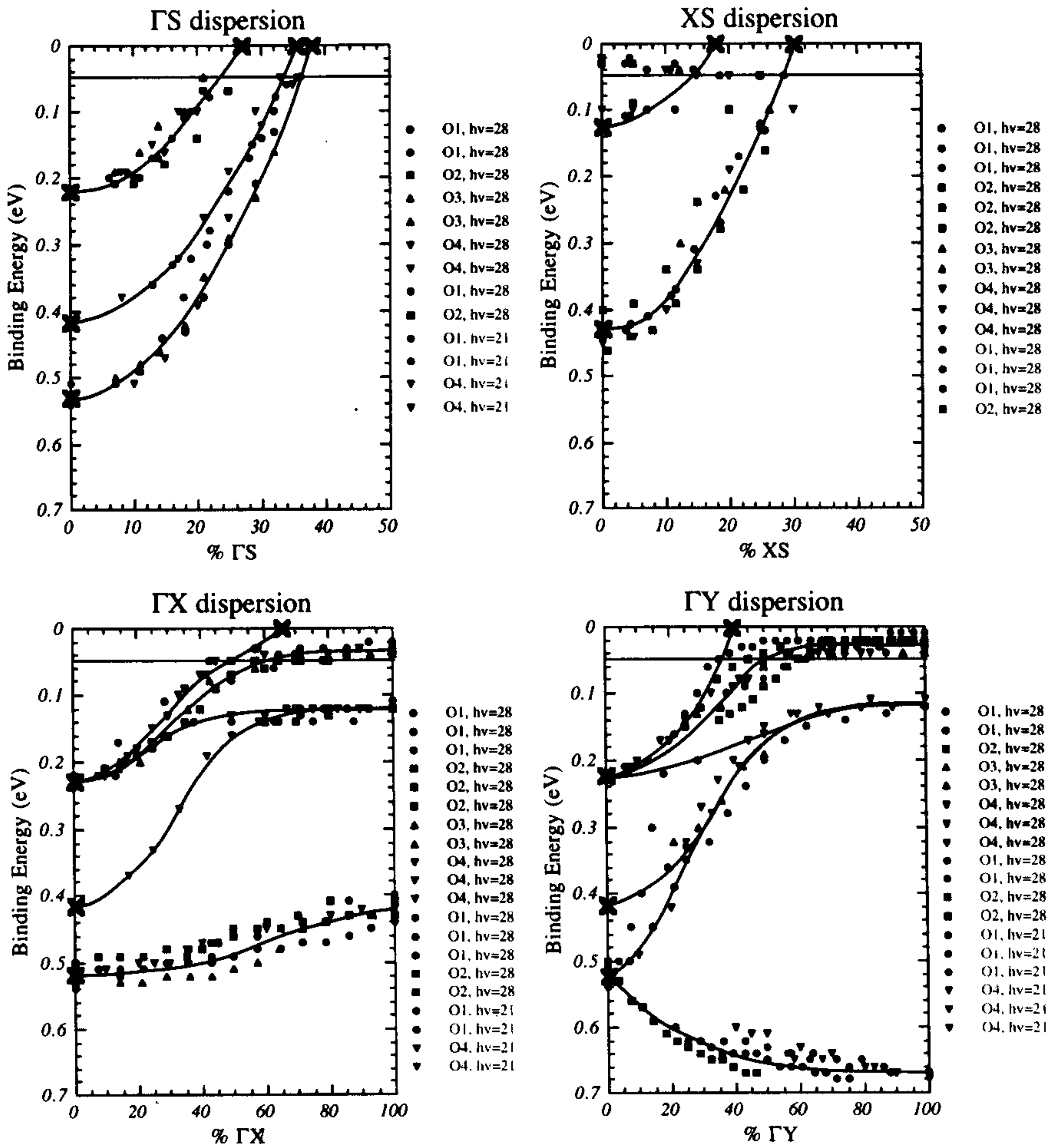






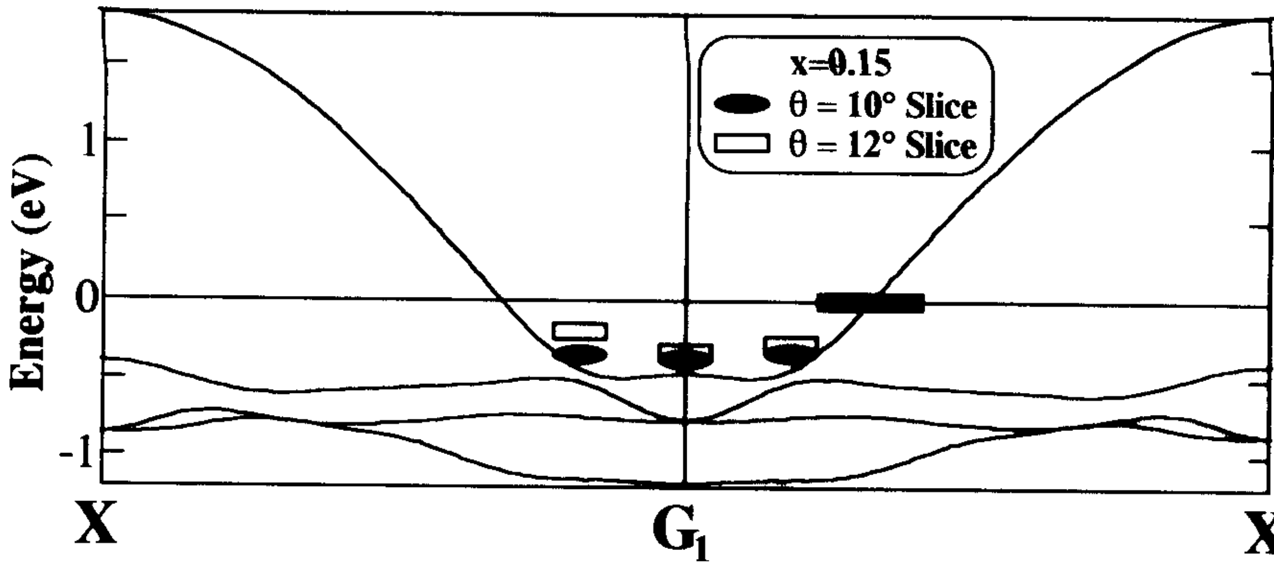


-0.8 -0.6 -0.4 -0.2 0 0.2
Optimal doping
O1 G-X
Optimal doping
O1 G-Y
Optimal doping
O1 G-S
Optimal doping
O1 X-Y
Optimal doping
O1 X-S
Optimal doping
O1 Y-S
Optimal doping
O2 G-X
Optimal doping
O2 G-Y
Optimal doping
O2 G-S
Optimal doping
O2 X-Y
Optimal doping
O2 X-S
Optimal doping
O2 Y-S
S Y S
X X
S Y S

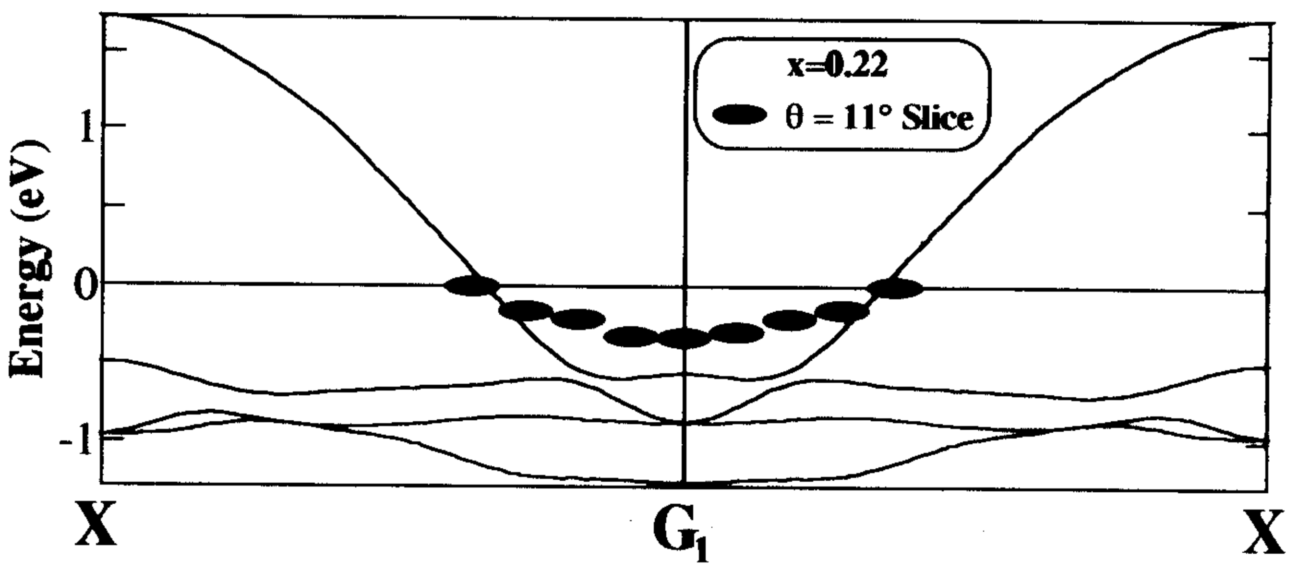


ΓS dispersion
Binding Energy (eV)
% ΓS
O1, hv=28
O1, hv=28
O2, hv=28
O3, hv=28
O3, hv=28
O4, hv=28
O4, hv=28
O1, hv=28
O2, hv=28
O1, hv=21
O1, hv=21
O4, hv=21
O4, hv=21
XS dispersion
Binding Energy (eV)
% XS
O1, hv=28
O1, hv=28
O1, hv=28
O2, hv=28
O2, hv=28
O2, hv=28
O3, hv=28
O3, hv=28
O4, hv=28
O4, hv=28
O4, hv=28
O1, hv=28
O1, hv=28
O1, hv=28
O2, hv=28
ΓX dispersion
Binding Energy (eV)
% ΓX
O1, hv=28
O1, hv=28
O1, hv=28
O2, hv=28
O2, hv=28
O2, hv=28
O3, hv=28
O3, hv=28
O4, hv=28
O4, hv=28
O4, hv=28
O1, hv=28
O1, hv=28
O1, hv=28
O2, hv=28
O2, hv=28
O1, hv=21
O1, hv=21
O4, hv=21
O4, hv=21
ΓY dispersion
Binding Energy (eV)
% ΓY
O1, hv=28
O1, hv=28
O2, hv=28
O3, hv=28
O3, hv=28
O4, hv=28
O4, hv=28
O4, hv=28
O1, hv=28
O1, hv=28
O2, hv=28
O2, hv=28
O1, hv=21
O1, hv=21
O1, hv=21
O4, hv=21
O4, hv=21
O4, hv=21

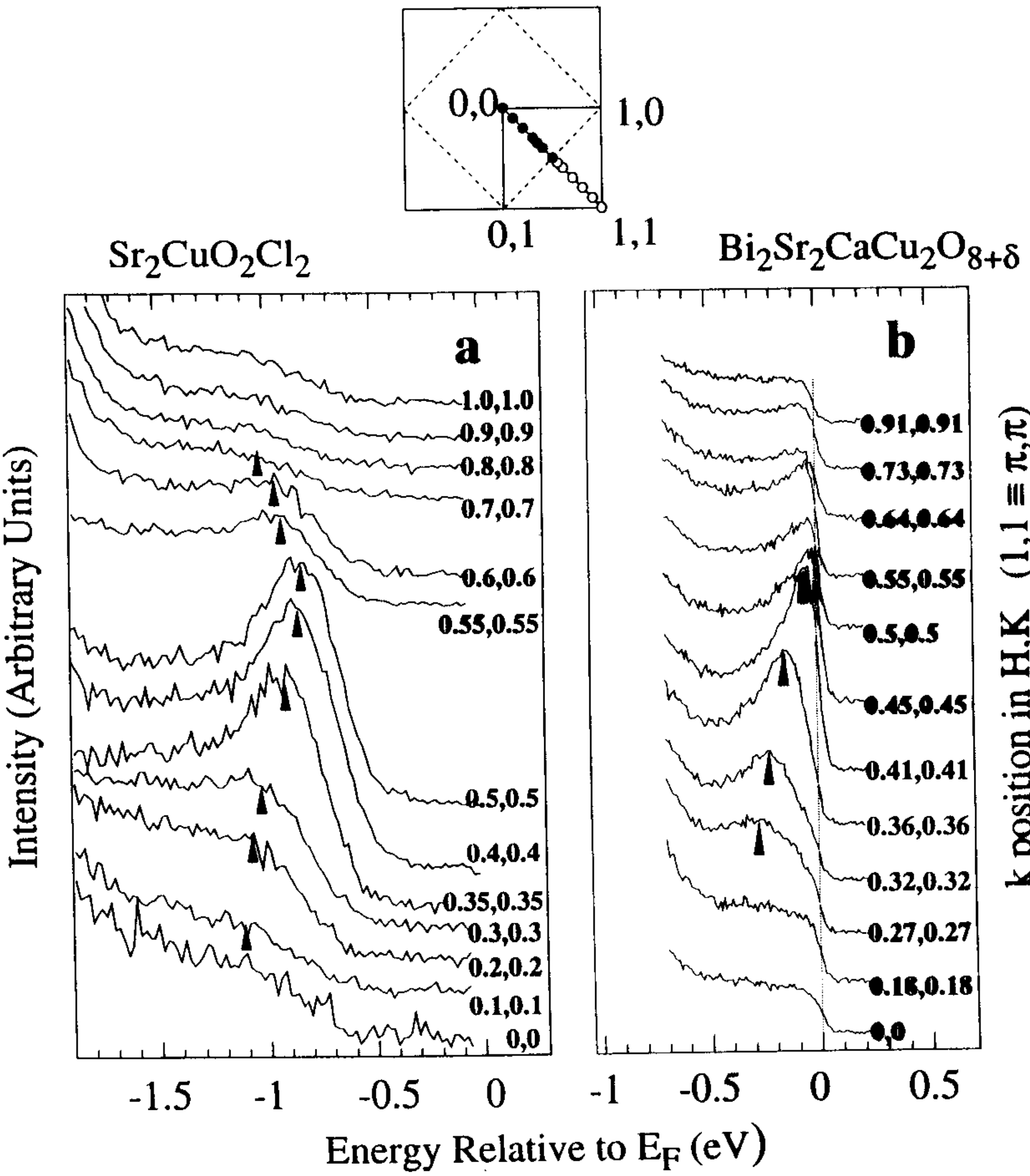
Band dispersion in $Nd_{1.85}Ce_{0.15}CuO_4$ along X-G_1-X



Band dispersion in $Nd_{1.78}Ce_{0.22}CuO_4$ along X-G_1-X

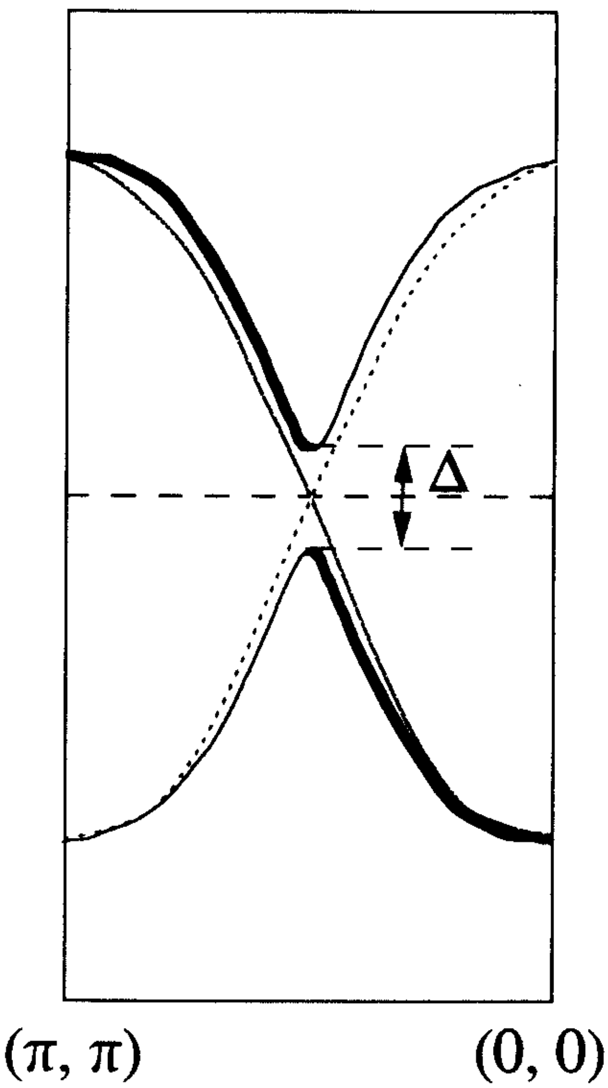


D.M. King, Z.-X. Shen, D.S. Dessau et al., Phys. Rev. Lett. 70, 3159 (1993)

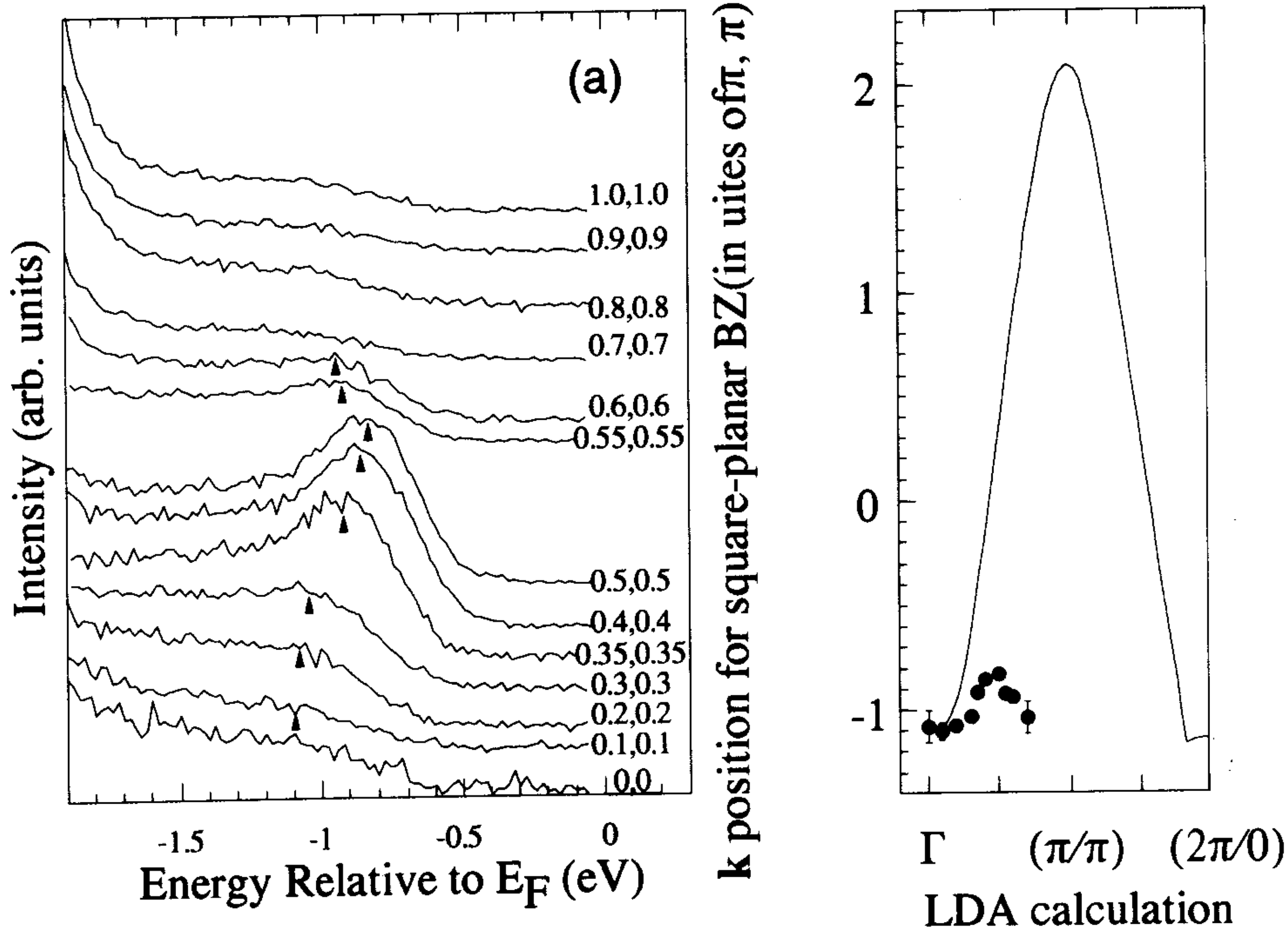


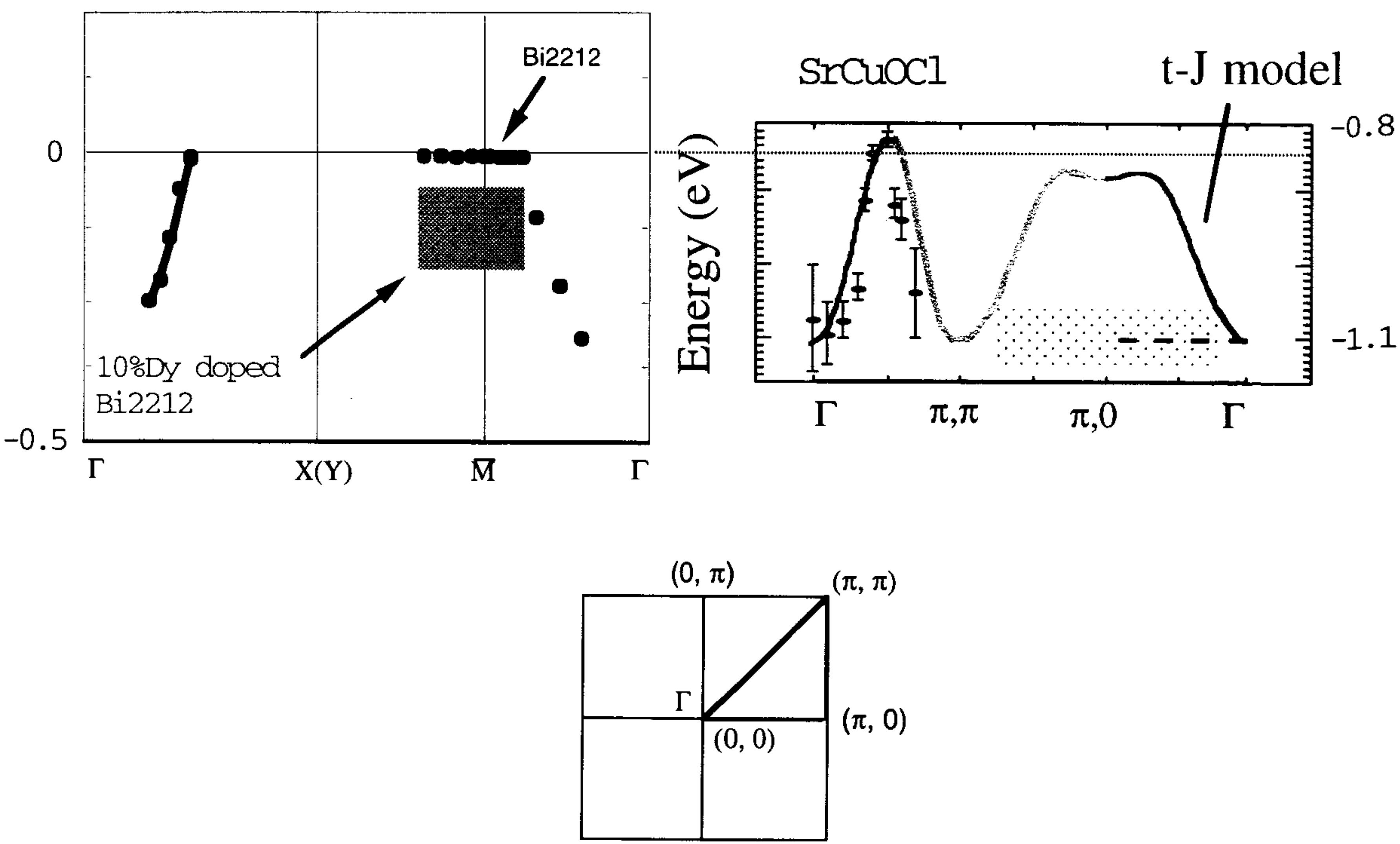
Wells, Shen, Matsuura, King, Kastner, Japsen,
Greven and Birgeneau. Phys. Rev. Lett. 74, 964 (1995).

Figure 1



Δ
(π, π)
(0, 0)


(a)
Intensity (arb. units)
1.0,1.0
0.9,0.9
0.8,0.8
0.7,0.7
0.6,0.6
0.55,0.55
0.5,0.5
0.4,0.4
0.35,0.35
0.3,0.3
0.2,0.2
0.1,0.1
0,0
-1.5
-1
-0.5
0
Energy Relative to E_F (eV)
k position for square-planar BZ(in uites ofπ, π)
2
1
0
-1
Γ
(π/π)
(2π/0)
LDA calculation



Bi2212
0
-0.5
10%Dy doped
Bi2212
Γ
X(Y)
M̄
Γ
SrCuOCl
t-J model
Energy (eV)
-0.8
-1.1
Γ
π,π
π,0
Γ
(0, π)
(π, π)
Γ
(π, 0)
(0, 0)

$SrCuO_2$ Structure

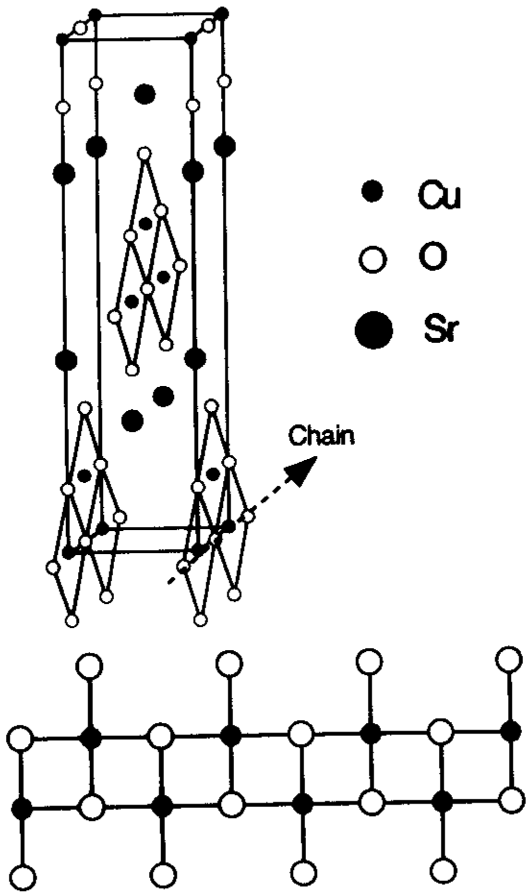
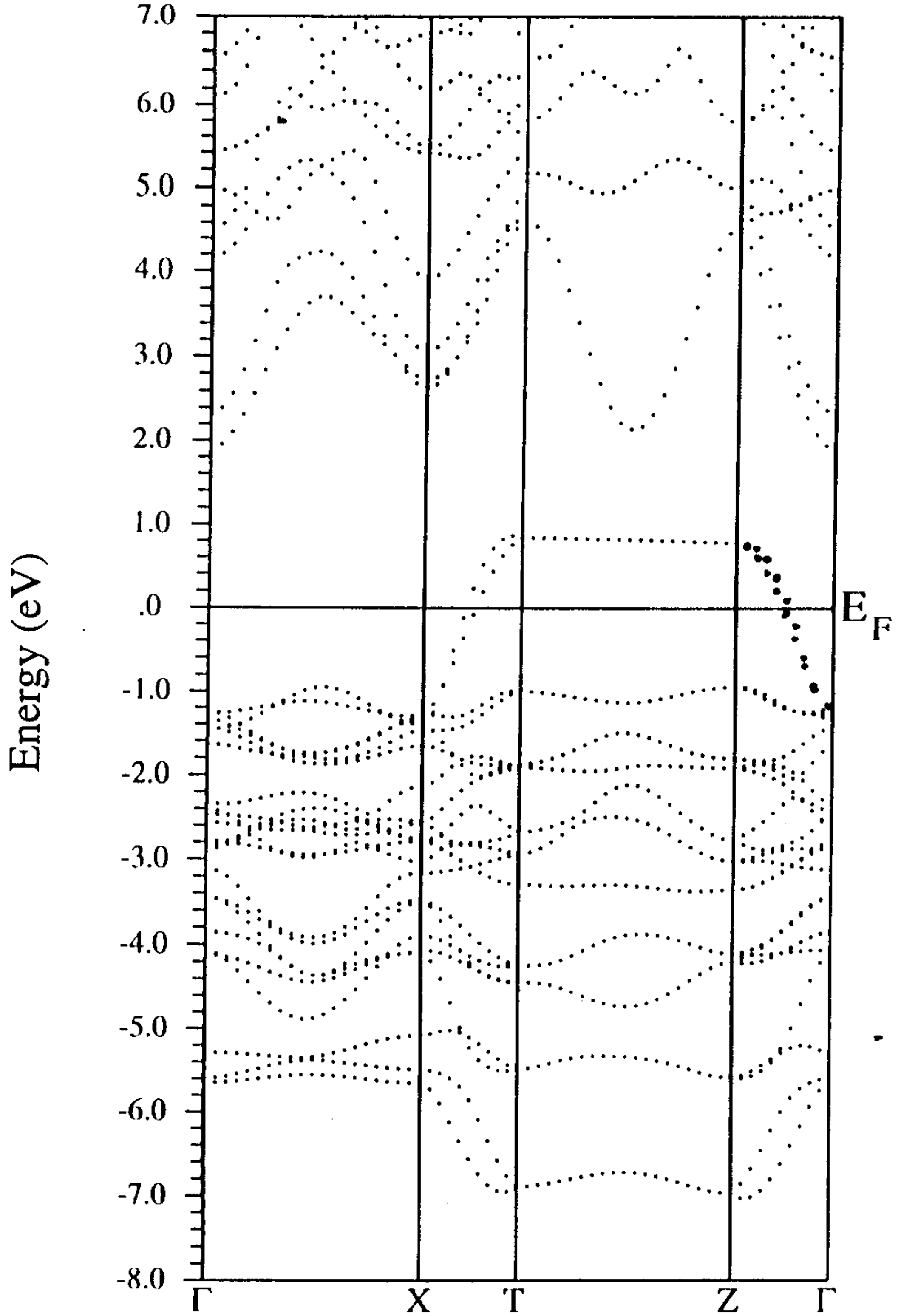
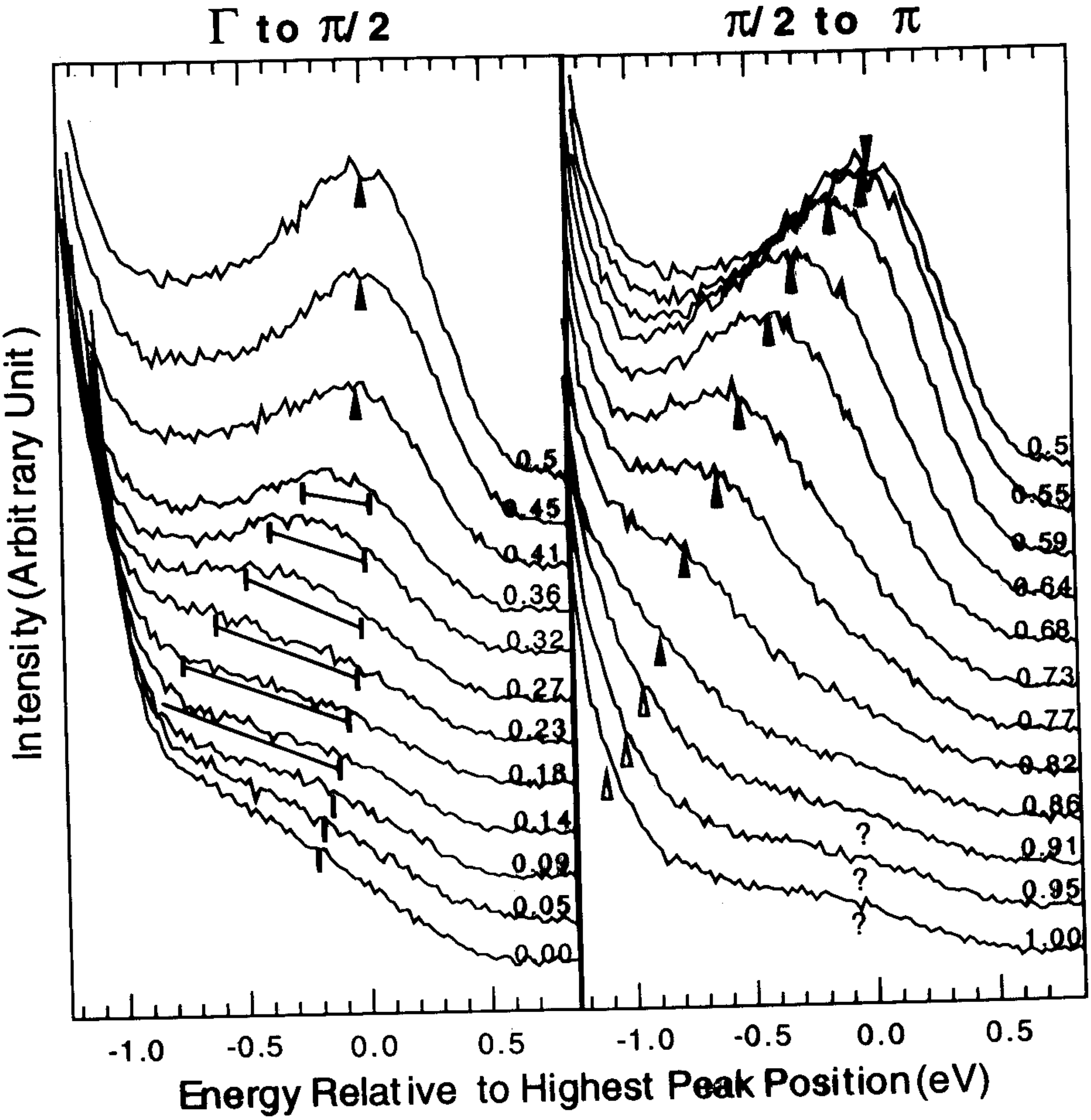


FIG. 2

SrCuO2 LDA (Peter Blaha)





Γ to π/2
π/2 to π
Intensity (Arbitrary Unit)
0.5
0.45
0.41
0.36
0.32
0.27
0.23
0.18
0.14
0.09
0.05
0.00
0.5
0.55
0.59
0.64
0.68
0.73
0.77
0.82
0.86
0.91
0.95
1.00
?
?
?
-1.0
-0.5
0.0
0.5
-1.0
-0.5
0.0
0.5
Energy Relative to Highest Peak Position (eV)

Figure 1.

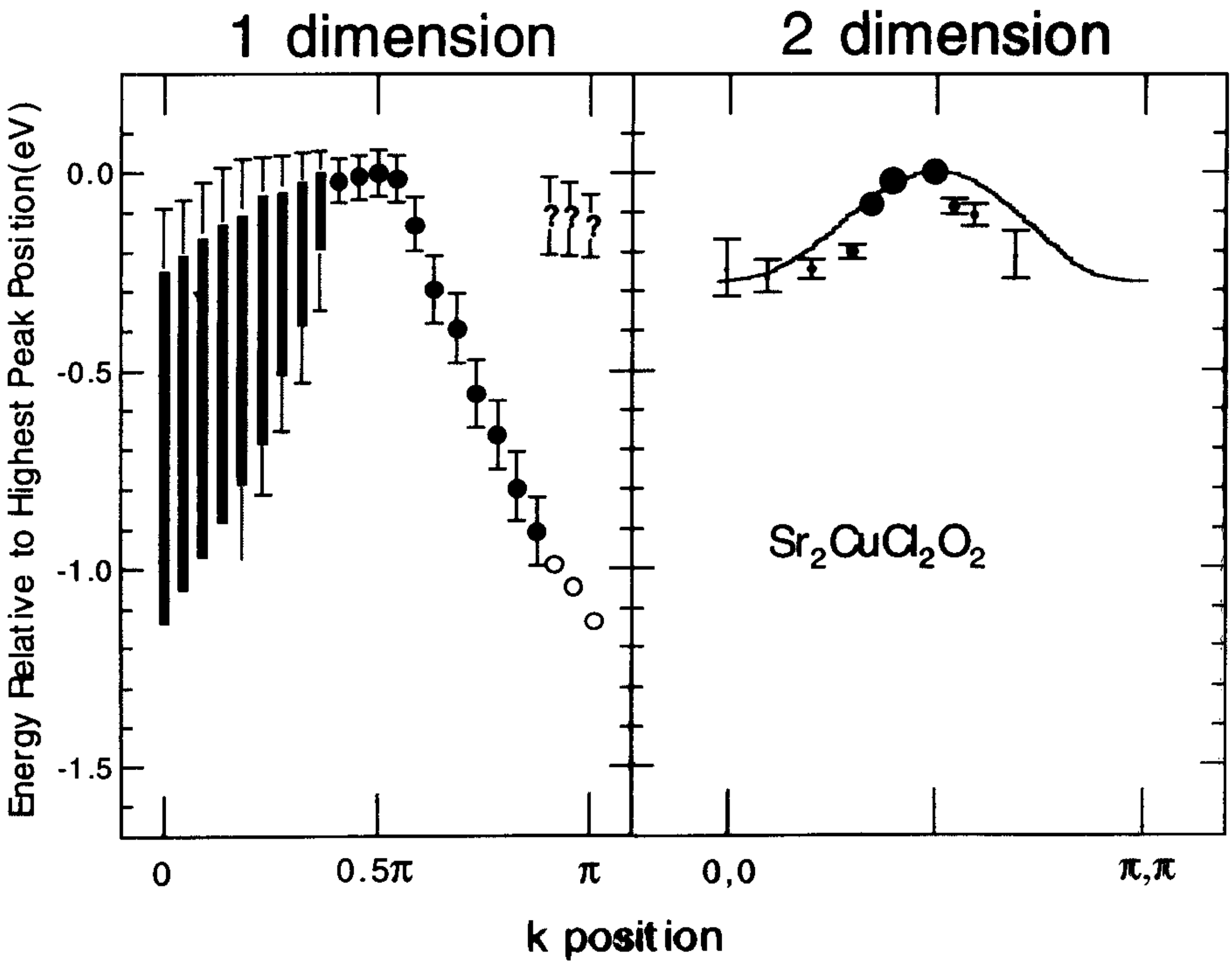
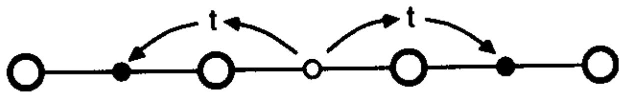

1 dimension
2 dimension
Energy Relative to Highest Peak Position(eV)
0.0
-0.5
-1.0
-1.5
???
$Sr_2CuCl_2O_2$
0
0.5π
π
0,0
π,π
k position

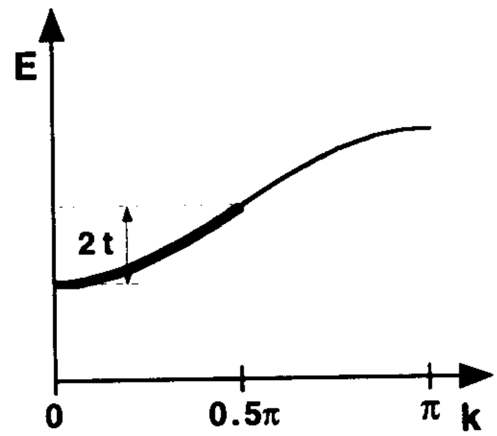
Figure 2.

Predicted Band Widths

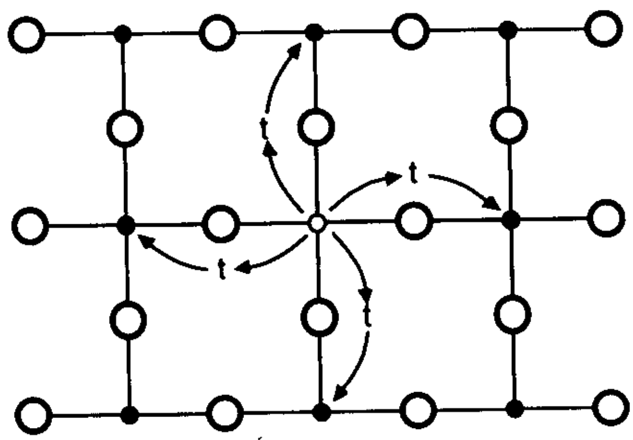
1 Dimension(Sr_2CuO_3, $SrCuO_2$,...)



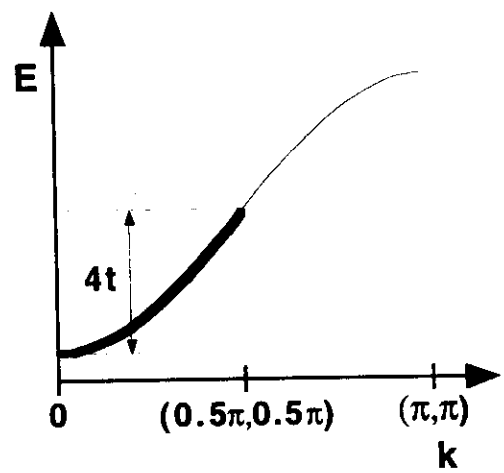
W = 2 t

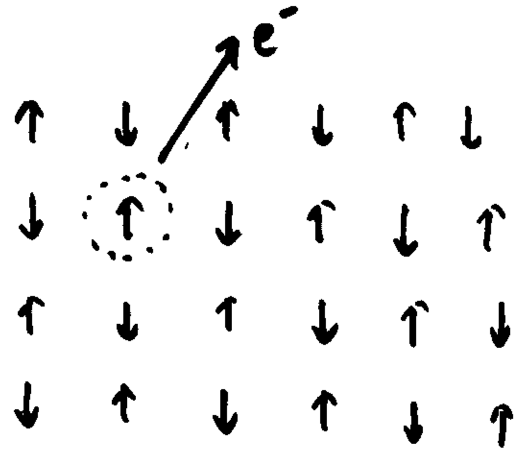


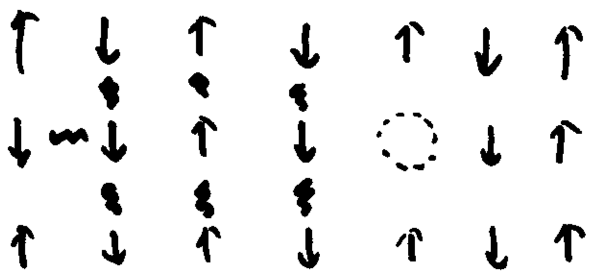
2 Dimension($Sr_2CuO_2Cl_2$, La_2CuO_4,...)

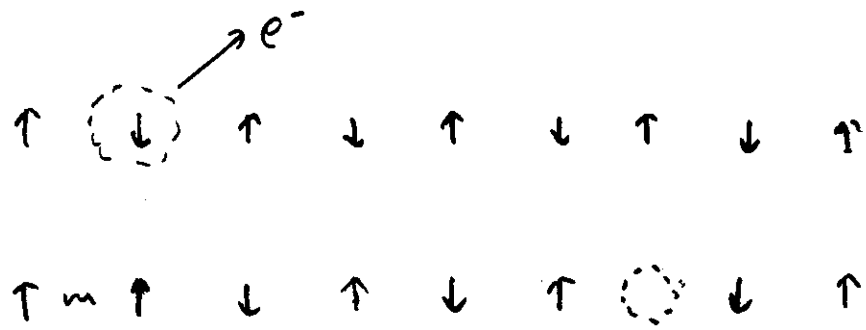


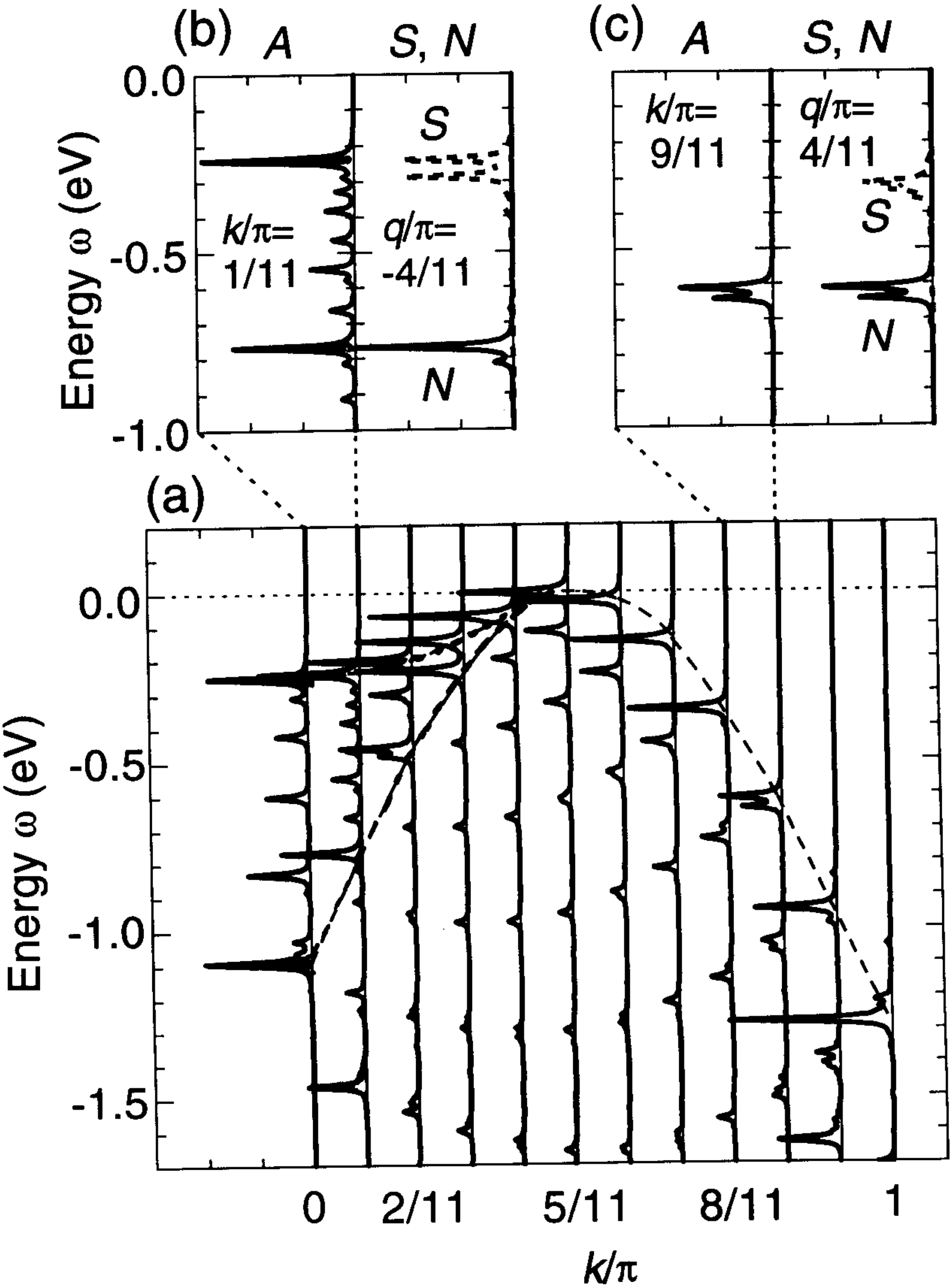
W = 4 t



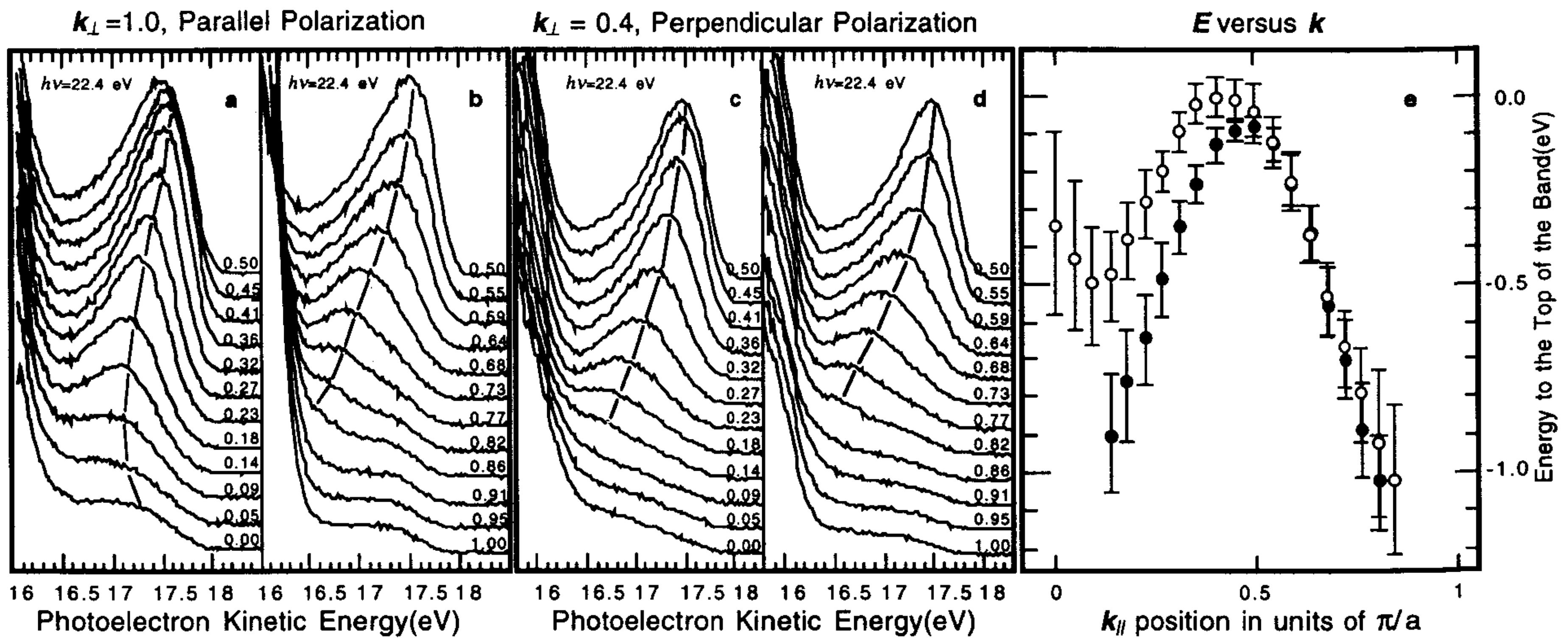

e^-




e^-



(b)
A
S, N
0.0
-0.5
-1.0
Energy ω (eV)
S
k/π=
1/11
q/π=
-4/11
N
(c)
A
S, N
k/π=
9/11
q/π=
4/11
S
N
(a)
0.0
-0.5
-1.0
-1.5
Energy ω (eV)
0
2/11
5/11
8/11
1
k/π



$k_\perp$ =1.0, Parallel Polarization
$k_\perp$ = 0.4, Perpendicular Polarization
E versus k
$h\nu$=22.4 eV
a
b
c
d
e
0.50
0.45
0.41
0.36
0.32
0.27
0.23
0.18
0.14
0.09
0.05
0.00
0.55
0.59
0.64
0.68
0.73
0.77
0.82
0.86
0.91
0.95
1.00
16 16.5 17 17.5 18
Photoelectron Kinetic Energy(eV)
0 0.5 1
$k_{//}$ position in units of π/a
0.0 -0.5 -1.0
Energy to the Top of the Band(eV)

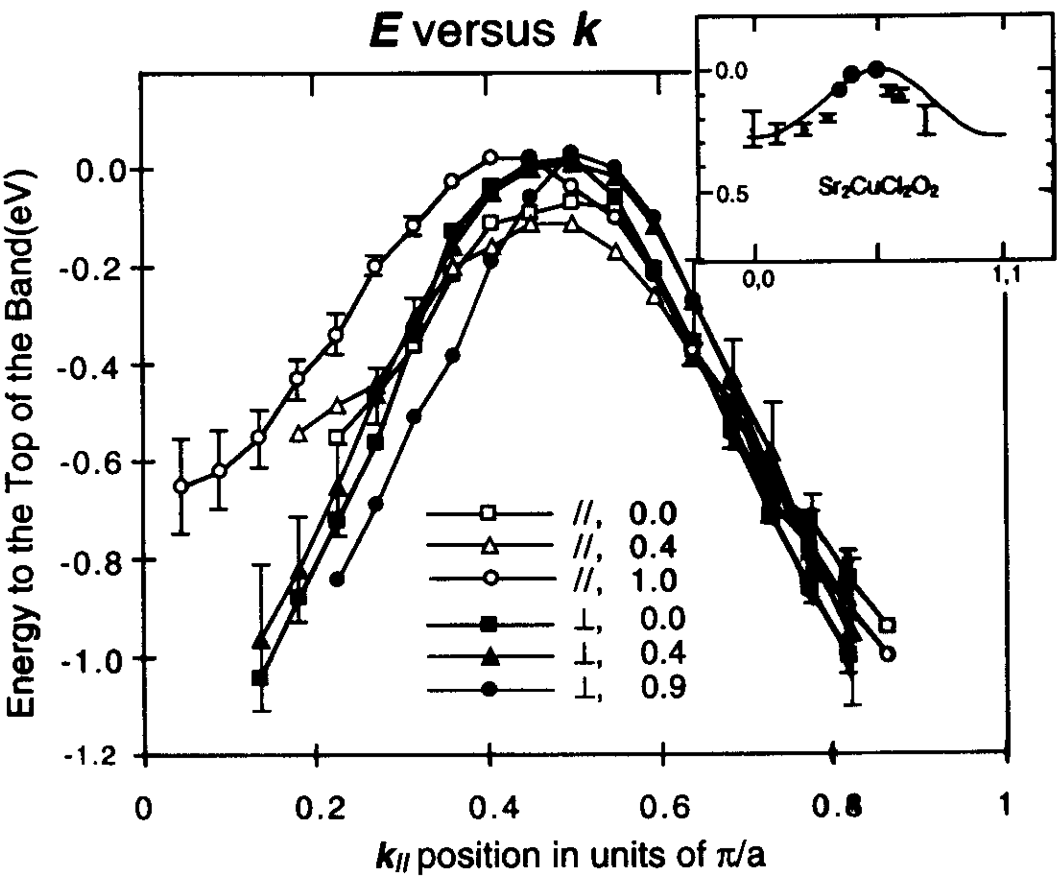
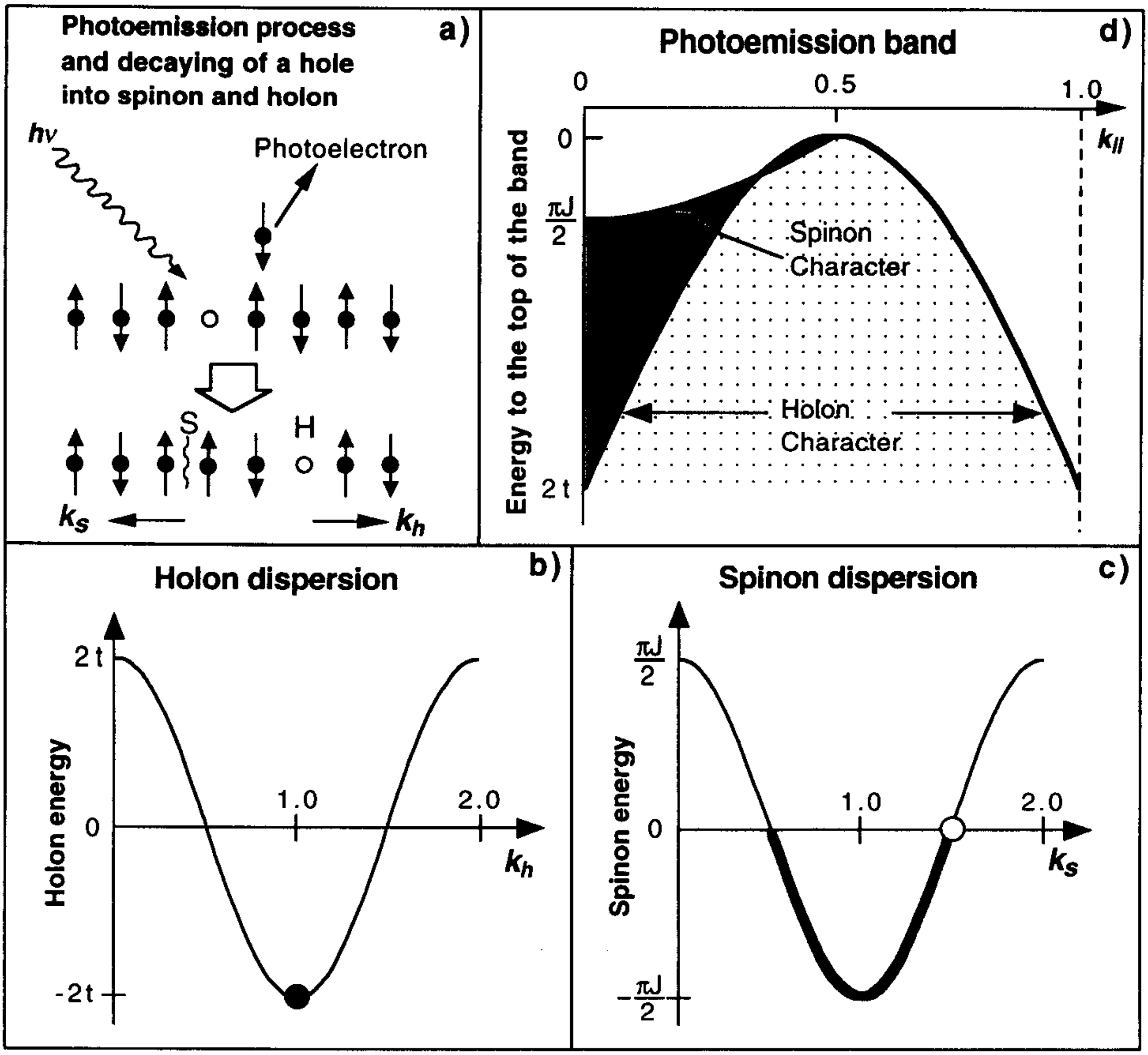

E versus k
Energy to the Top of the Band(eV)
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
0
0.2
0.4
0.6
0.8
1
$k_{//}$ position in units of π/a
//, 0.0
//, 0.4
//, 1.0
⊥, 0.0
⊥, 0.4
⊥, 0.9
0.0
0.5
0,0
1,1
$Sr_2CuCl_2O_2$

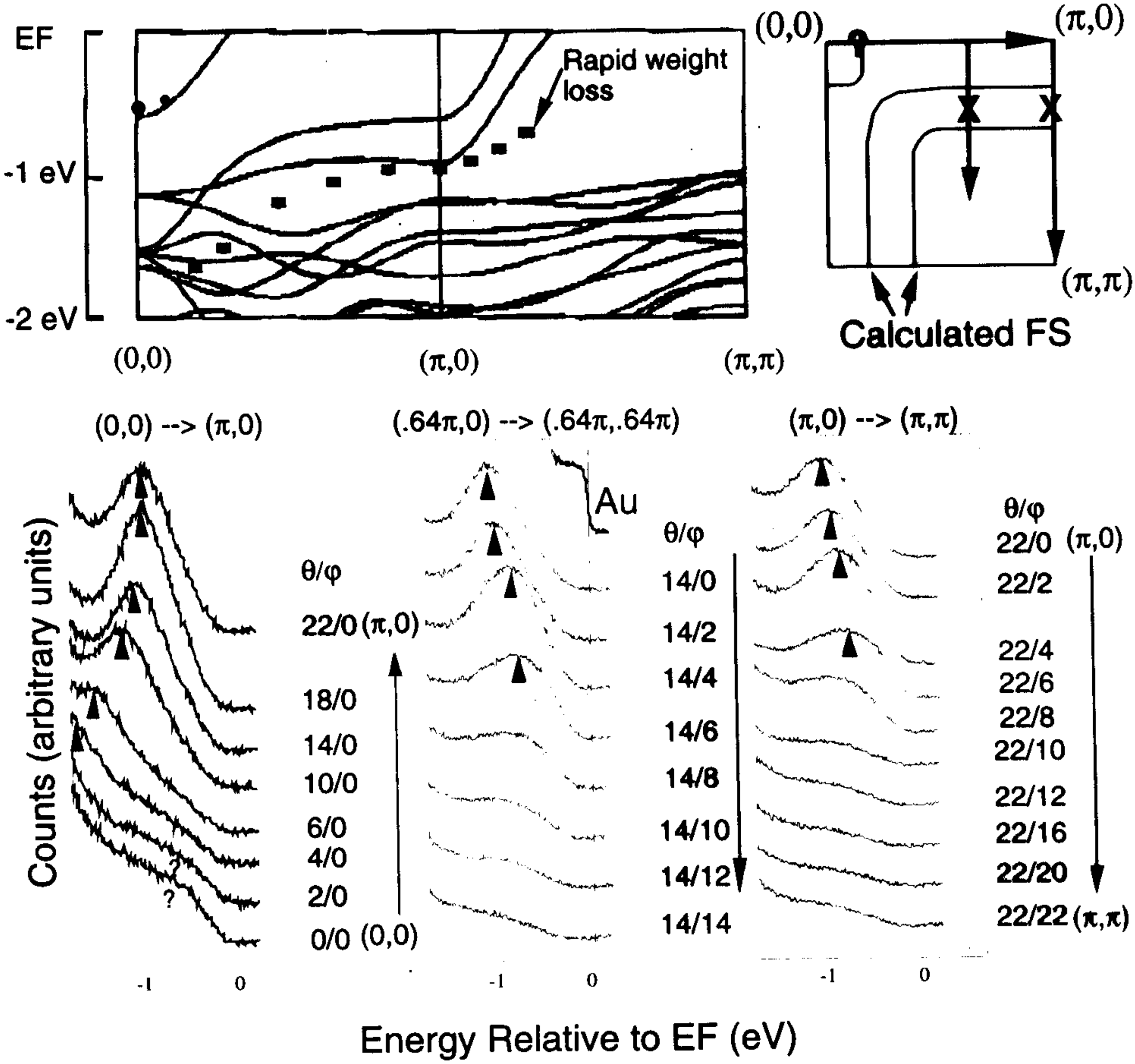
FIG. 5

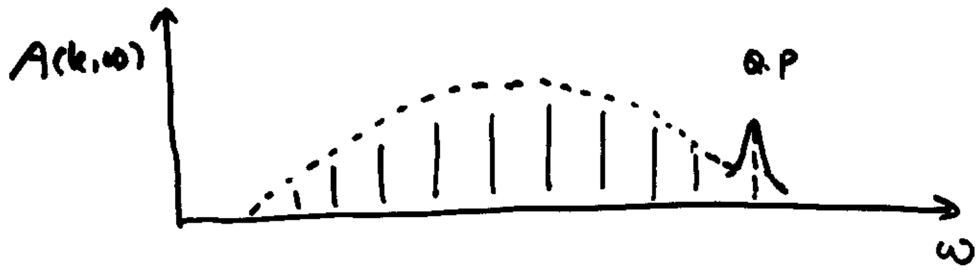


Photoemission process
and decaying of a hole
into spinon and holon
a)
hν
Photoelectron
S
H
k_s
k_h
Photoemission band
d)
0
0.5
1.0
$k_{//}$
Energy to the top of the band
0
$\frac{\pi J}{2}$
2t
Spinon
Character
Holon
Character
Holon dispersion
b)
2t
0
-2t
1.0
2.0
k_h
Holon energy
Spinon dispersion
c)
$\frac{\pi J}{2}$
0
$-\frac{\pi J}{2}$
1.0
2.0
k_s
Spinon energy

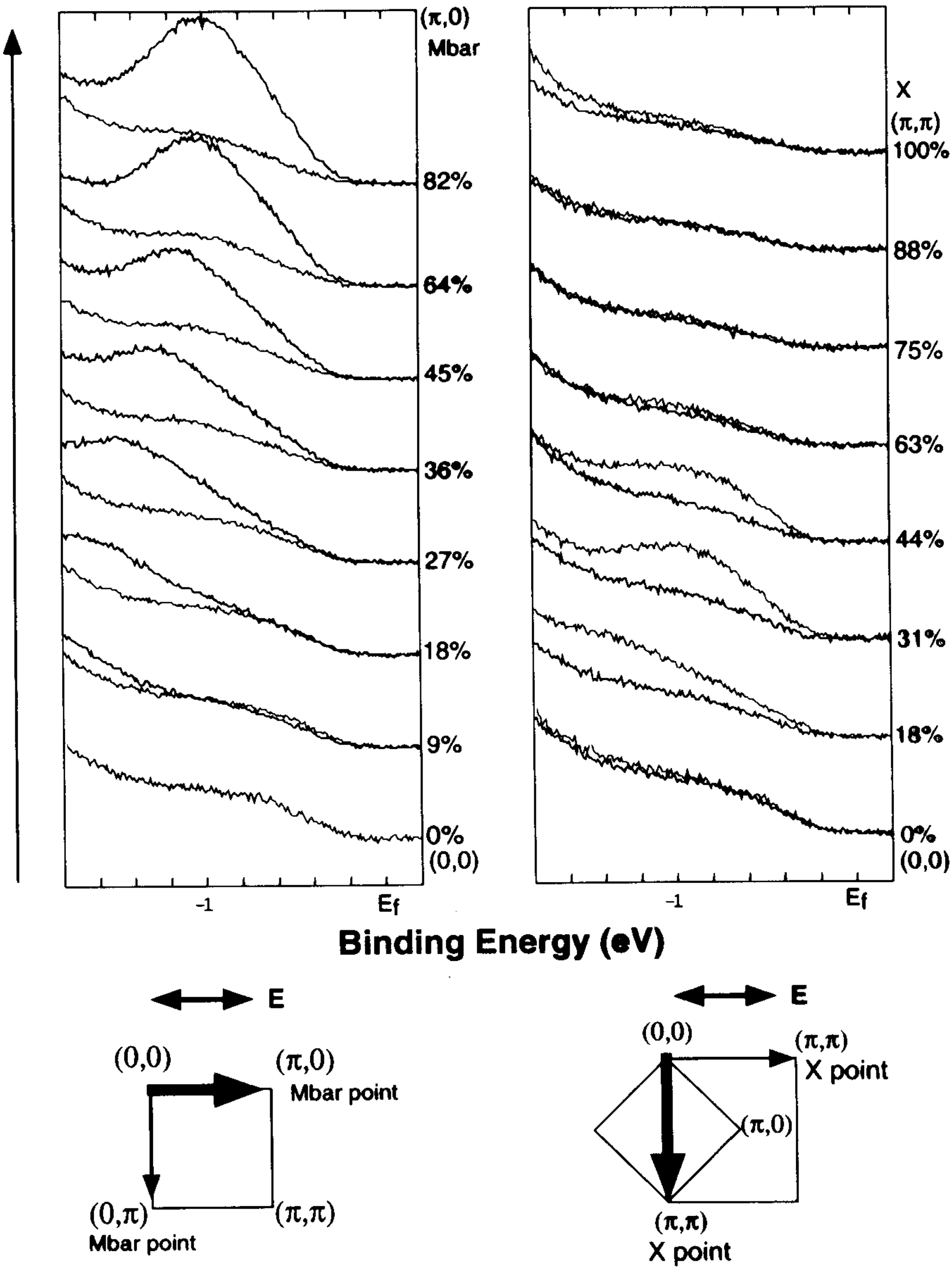
Peak Centroids vs. LSDA band calculation results
(Ferromagnetic up-spin bands)
Calculation by N. Hamada

La1.2Sr1.8Mn2O7 (x=.4) 2 layer manganite
Measurement at T=10K hv=22.4 eV

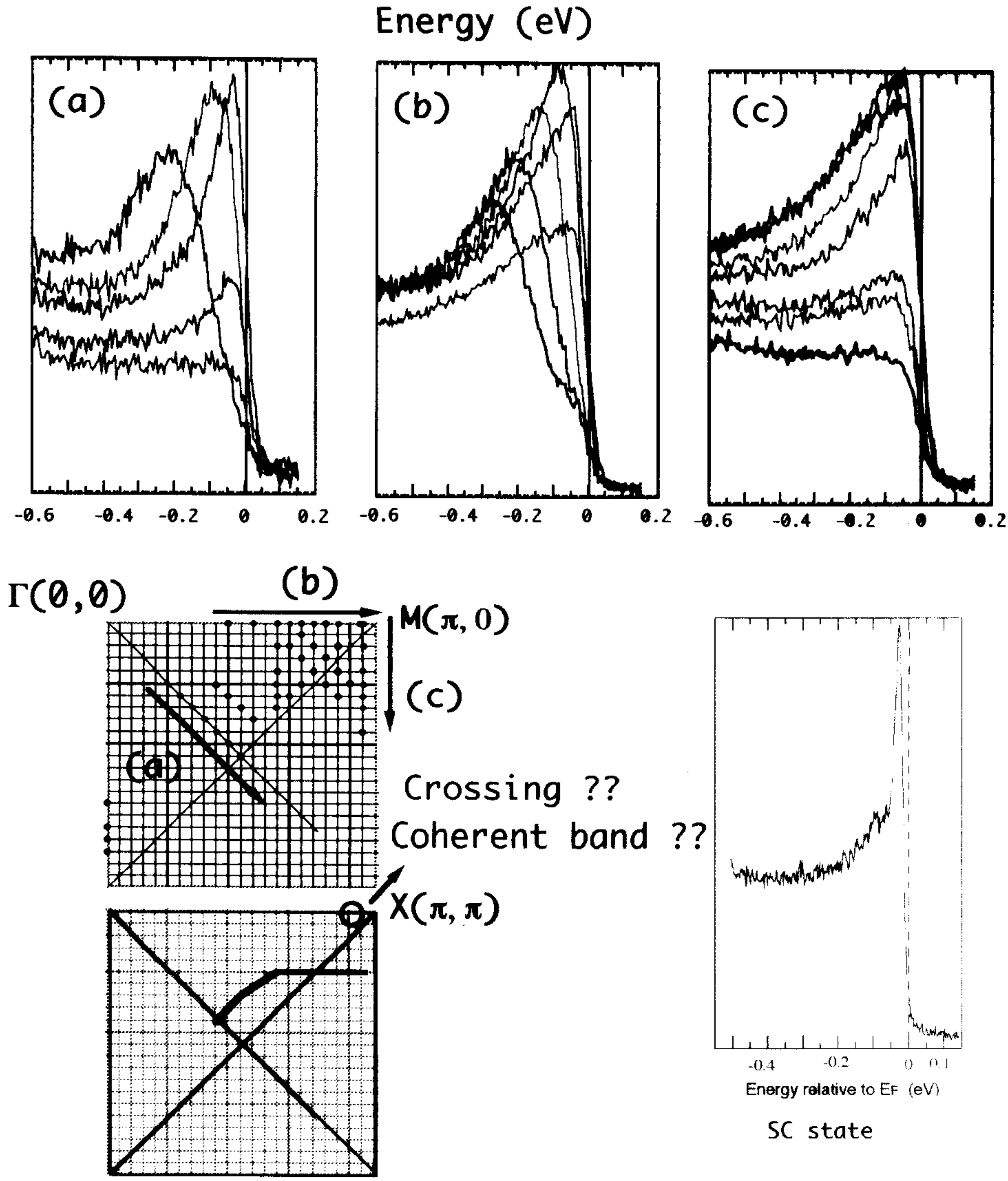


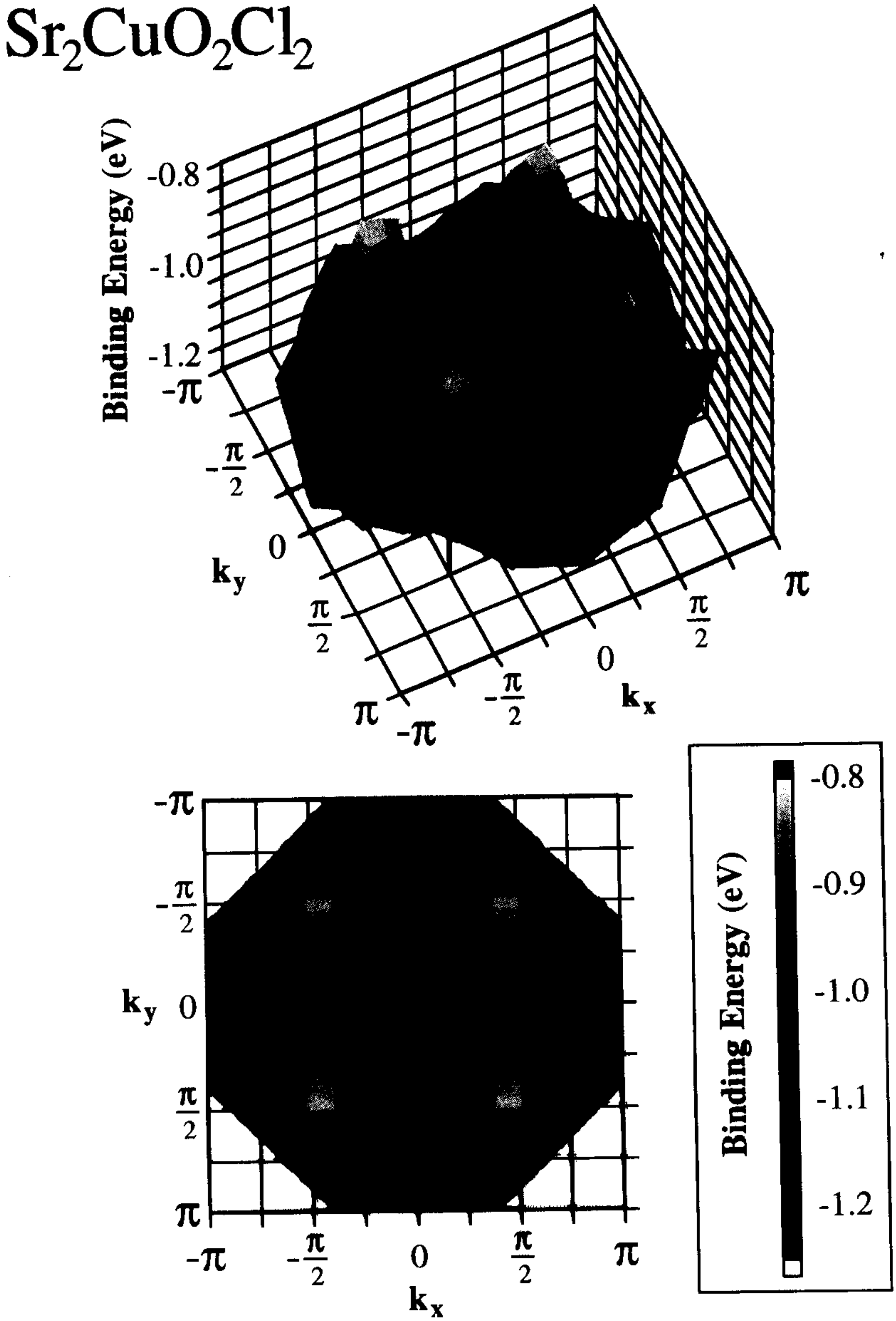

A(k,ω)
Q.P
ω

Polarization and symmetry study of 2layer $d^{3.6}$ manganite

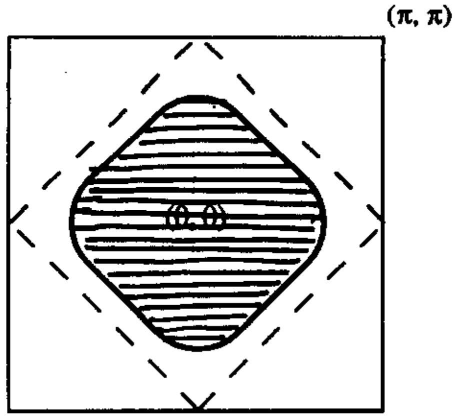


94-36 2212 600 Air Anneal (Tc =85K)

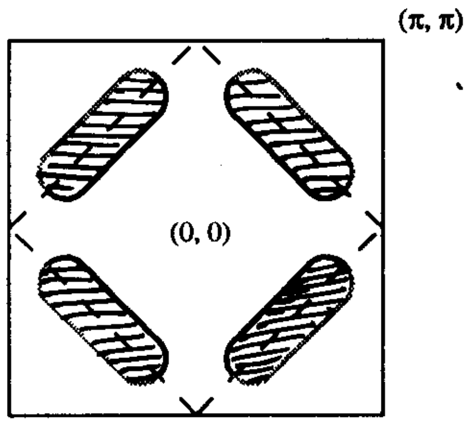




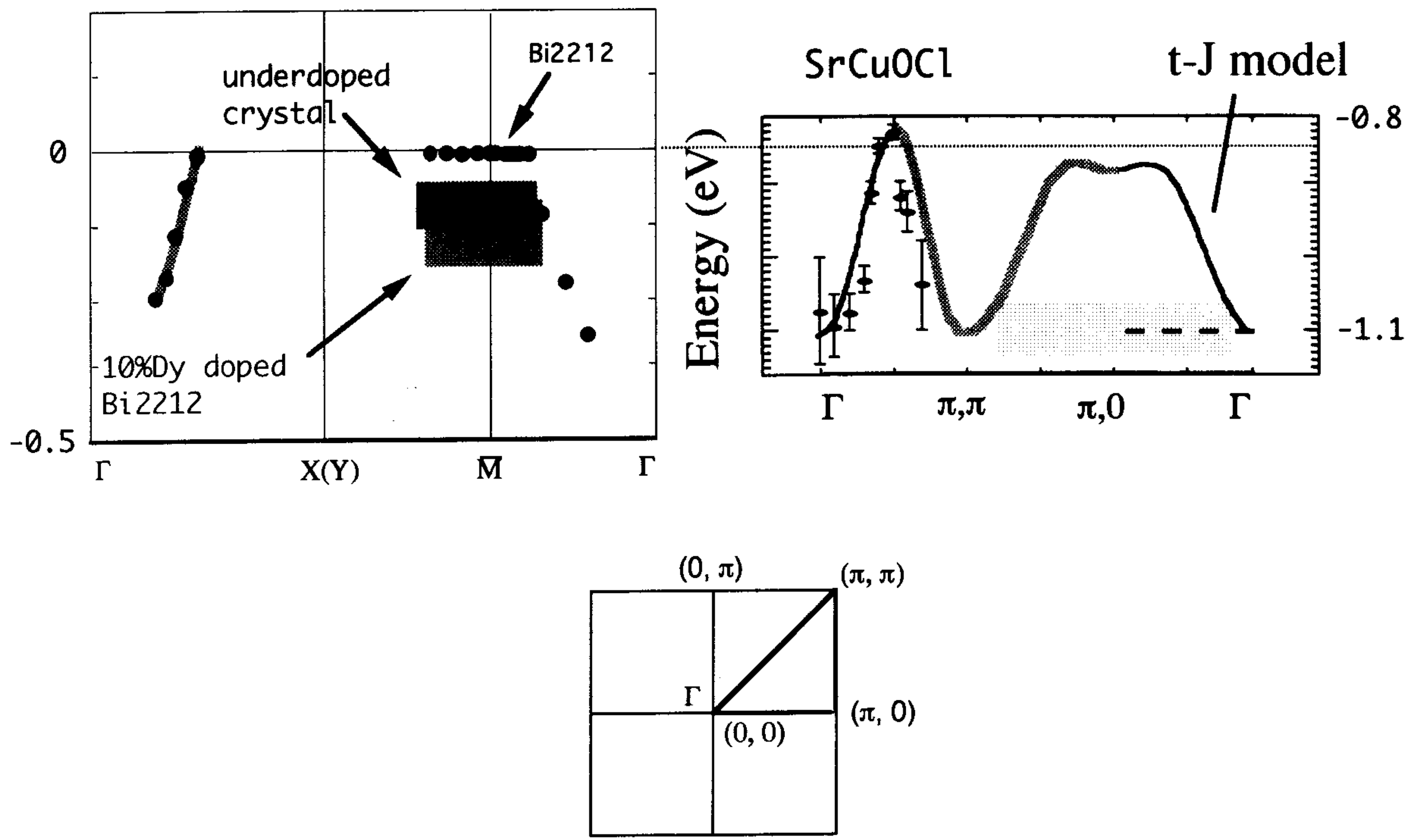
$Sr_2CuO_2Cl_2$
Binding Energy (eV)
-0.8
-1.0
-1.2
$-\pi$
$-\frac{\pi}{2}$
0
k_y
$\frac{\pi}{2}$
π
$-\pi$
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π
k_x
$-\pi$
$-\frac{\pi}{2}$
k_y 0
$\frac{\pi}{2}$
π
$-\pi$
$-\frac{\pi}{2}$
0
$\frac{\pi}{2}$
π
k_x
Binding Energy (eV)
-0.8
-0.9
-1.0
-1.1
-1.2



band FS



"Many-body" FS



underdoped
crystal
Bi2212
10%Dy doped
Bi2212
0
-0.5
Γ
X(Y)
M̄
Γ
SrCuOCl
t-J model
Energy (eV)
-0.8
-1.1
Γ
π,π
π,0
Γ
(0, π)
(π, π)
Γ
(π, 0)
(0, 0)

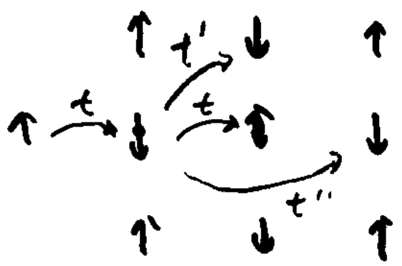
Requirement for a theoretical model:

* Dispersion of metal
  (Note $t-J$)

* Dispersion of the insulator
  (Note $t-t'-t''-J$)

Evolution?

Eder, Otha, Sawatzky



* Lineshape (Kim, Shen, Tohyama, Maekawa ..)

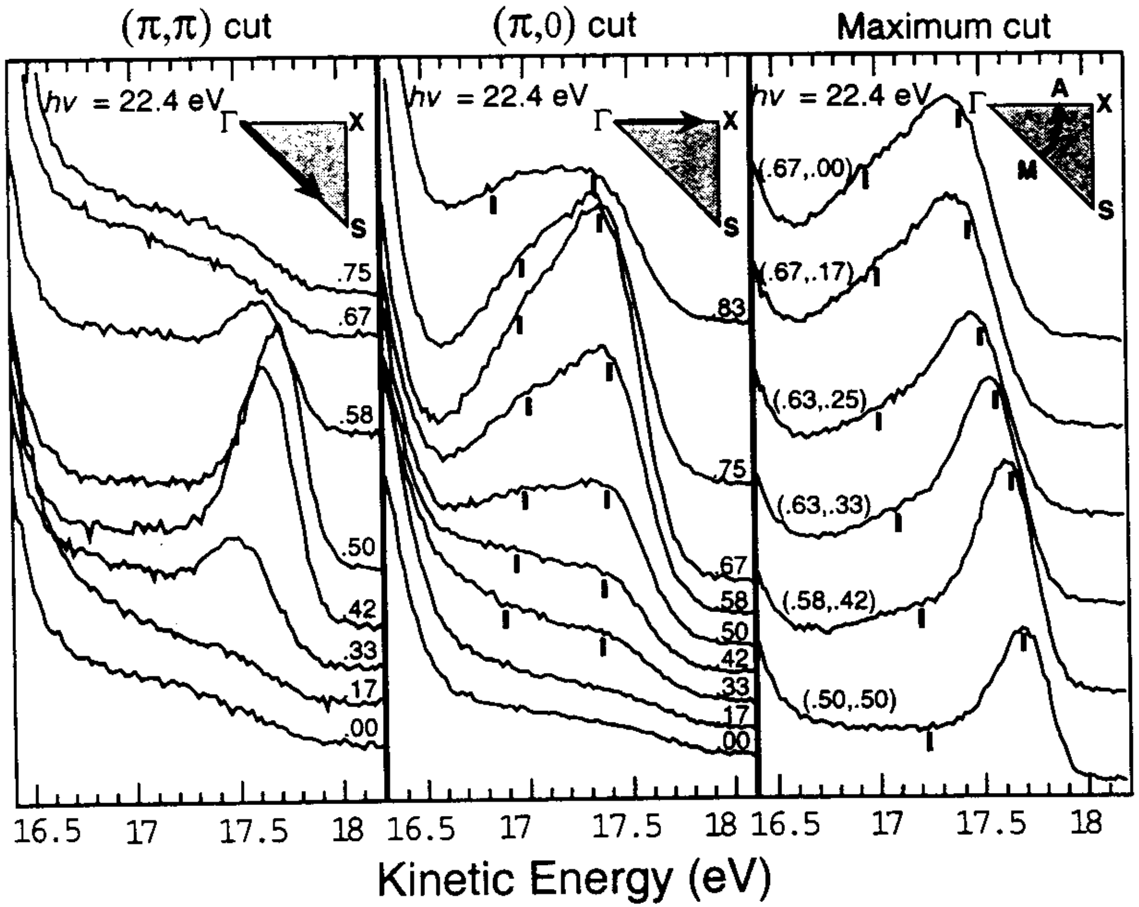

(π,π) cut
(π,0) cut
Maximum cut
hv = 22.4 eV
Γ
X
S
A
M
.75
.67
.58
.50
.42
.33
.17
.00
.83
(.67,.00)
(.67,.17)
(.63,.25)
(.63,.33)
(.58,.42)
(.50,.50)
16.5
17
17.5
18
Kinetic Energy (eV)

Figure 1

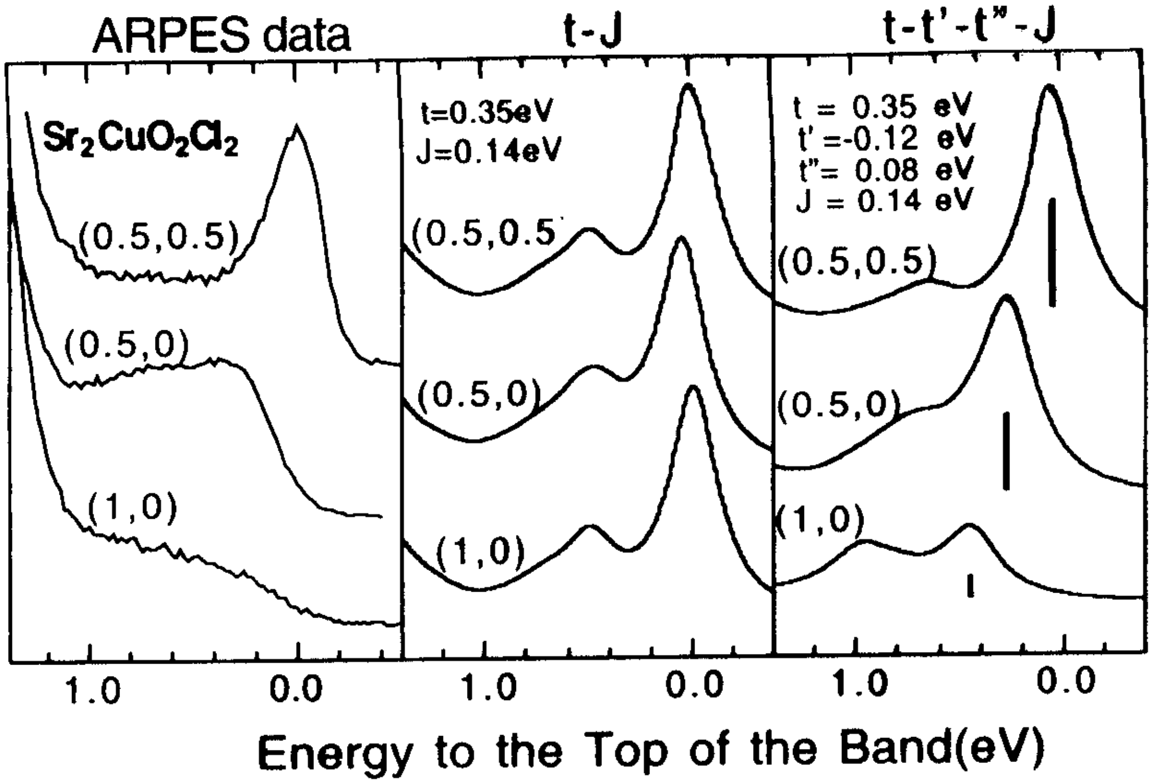

ARPES data
t-J
t-t'-t"-J
Sr2CuO2Cl2
(0.5,0.5)
(0.5,0)
(1,0)
t=0.35eV
J=0.14eV
t = 0.35 eV
t' =-0.12 eV
t"= 0.08 eV
J = 0.14 eV
1.0
0.0
Energy to the Top of the Band(eV)

Figure 2

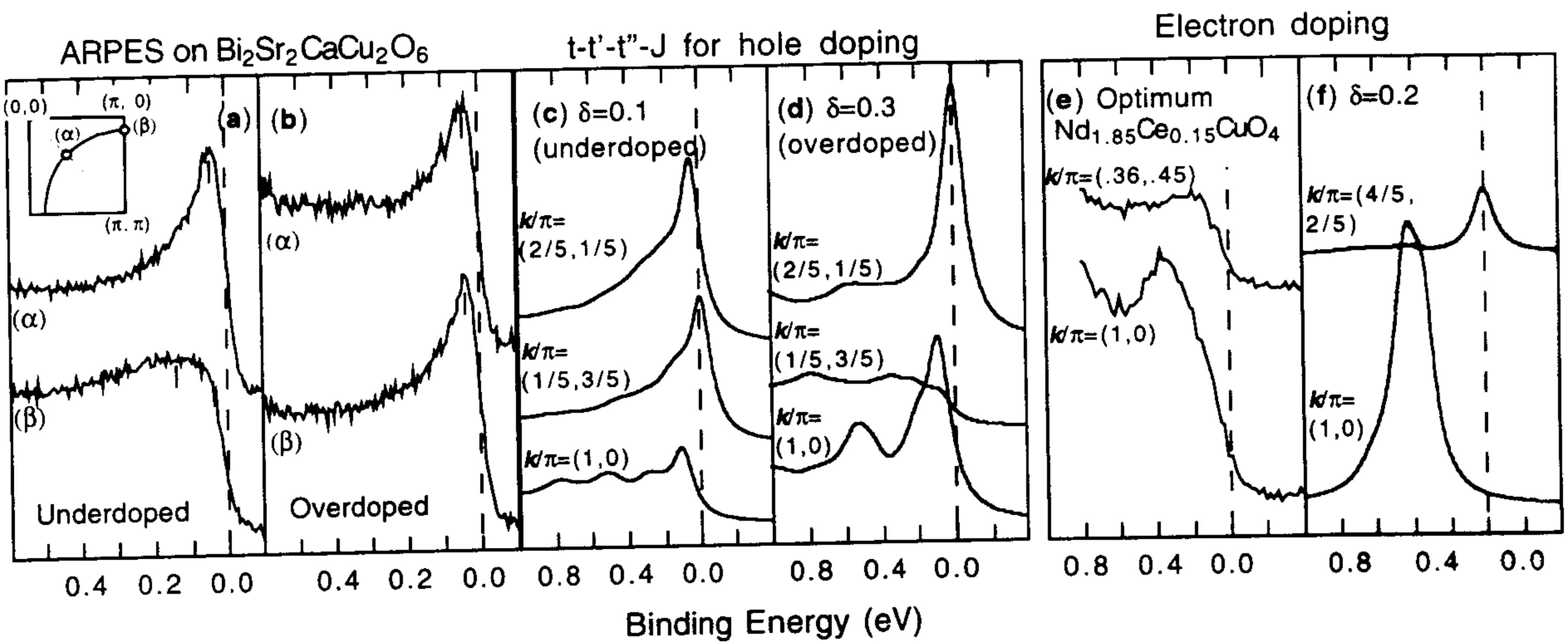

ARPES on Bi2Sr2CaCu2O6
t-t'-t"-J for hole doping
Electron doping
(a)
(b)
(c) δ=0.1
(underdoped)
(d) δ=0.3
(overdoped)
(e) Optimum
Nd1.85Ce0.15CuO4
(f) δ=0.2
(0,0)
(π, 0)
(π, π)
(α)
(β)
Underdoped
Overdoped
k/π=(2/5,1/5)
k/π=(1/5,3/5)
k/π=(1,0)
k/π=(.36,.45)
k/π=(4/5, 2/5)
0.4 0.2 0.0
0.8 0.4 0.0
Binding Energy (eV)

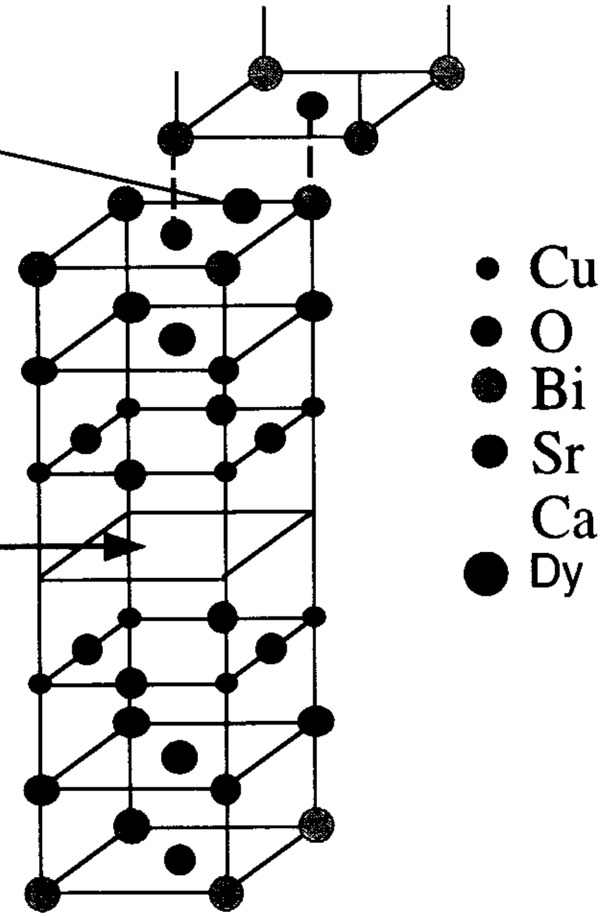
Figure 3

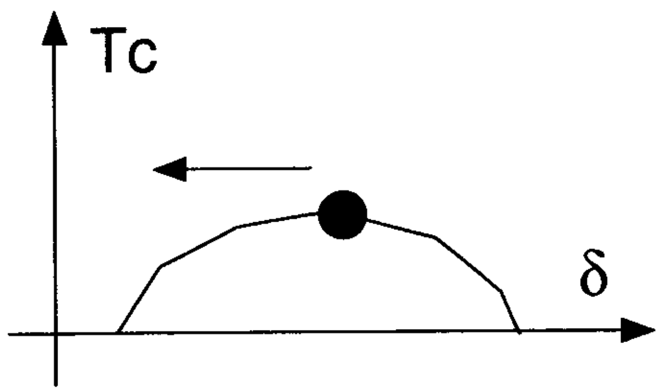
Two ways to underdope Bi2212

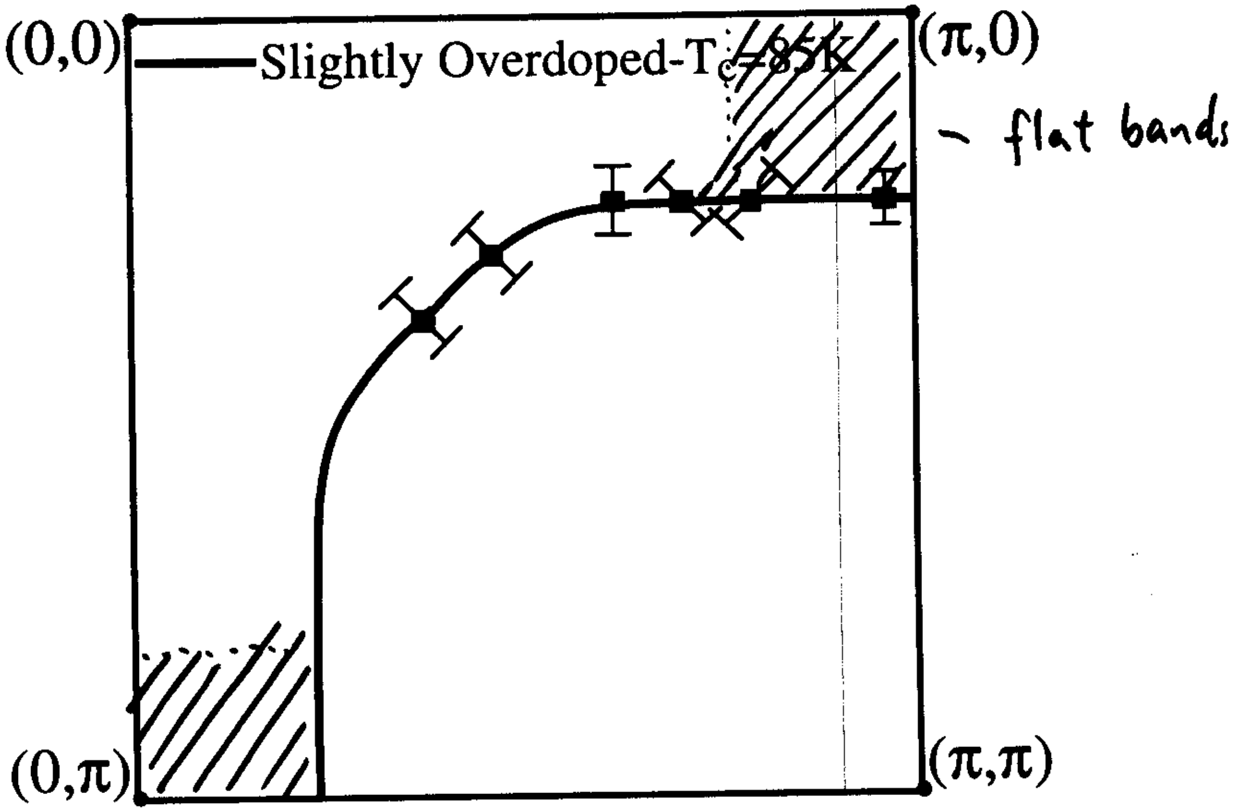
(Very different structural side effects)

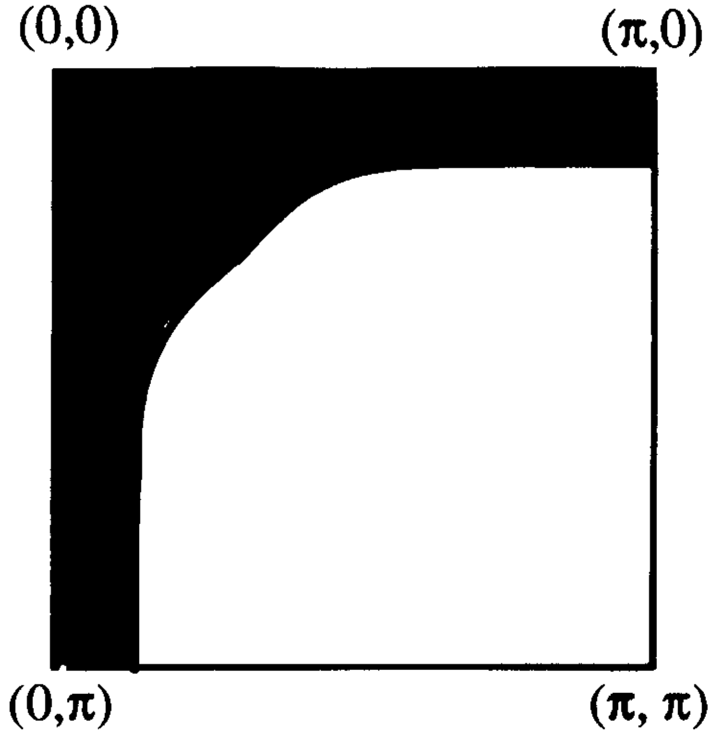
(i) Oxygen removal

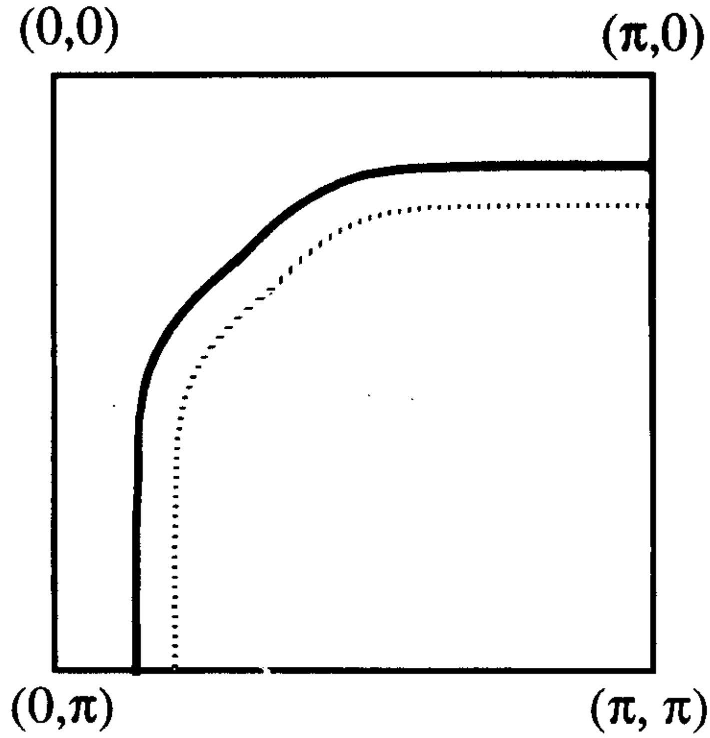
(ii) Dy/Ca substitution

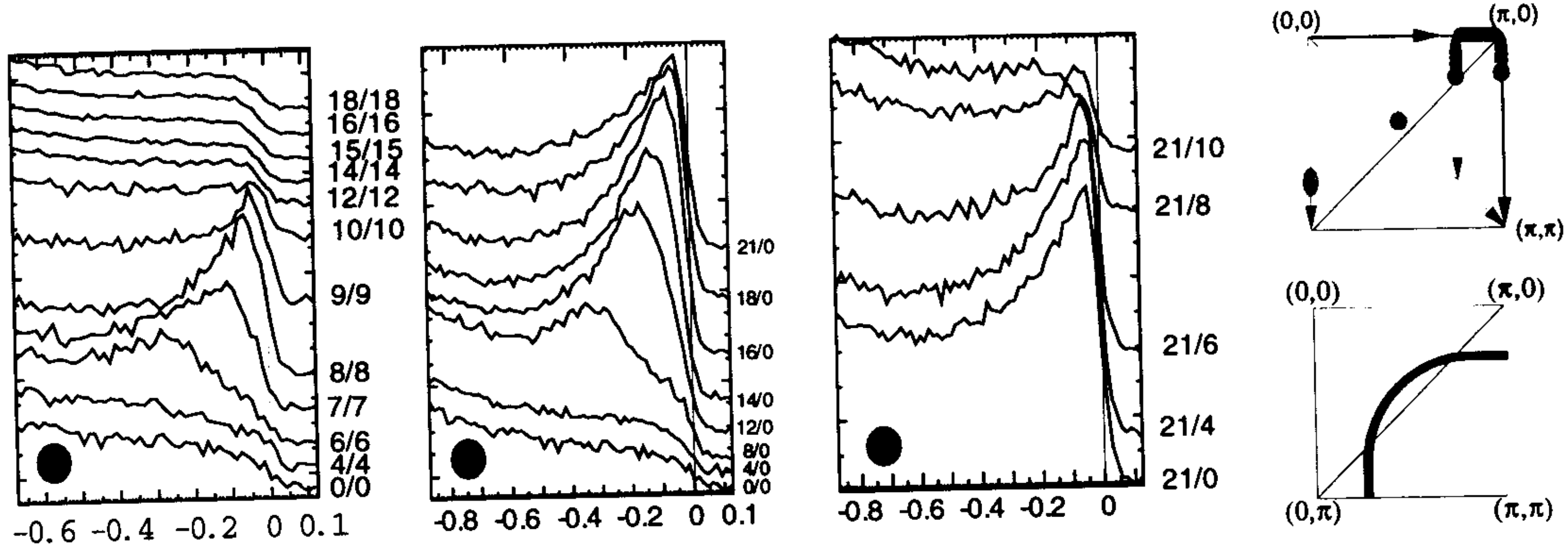




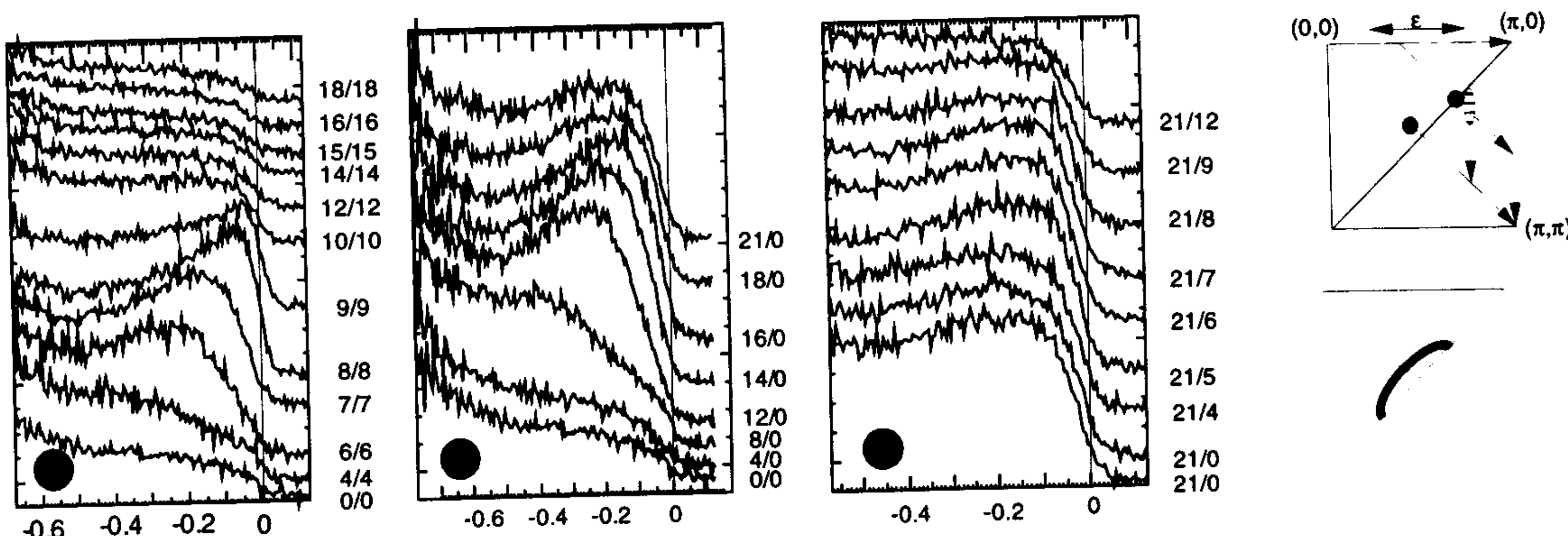

(0,0)
Slightly Overdoped-T_c=85K
(π,0)
flat bands
(0,π)
(π,π)


(0,0)
(π,0)
(0,π)
(π, π)

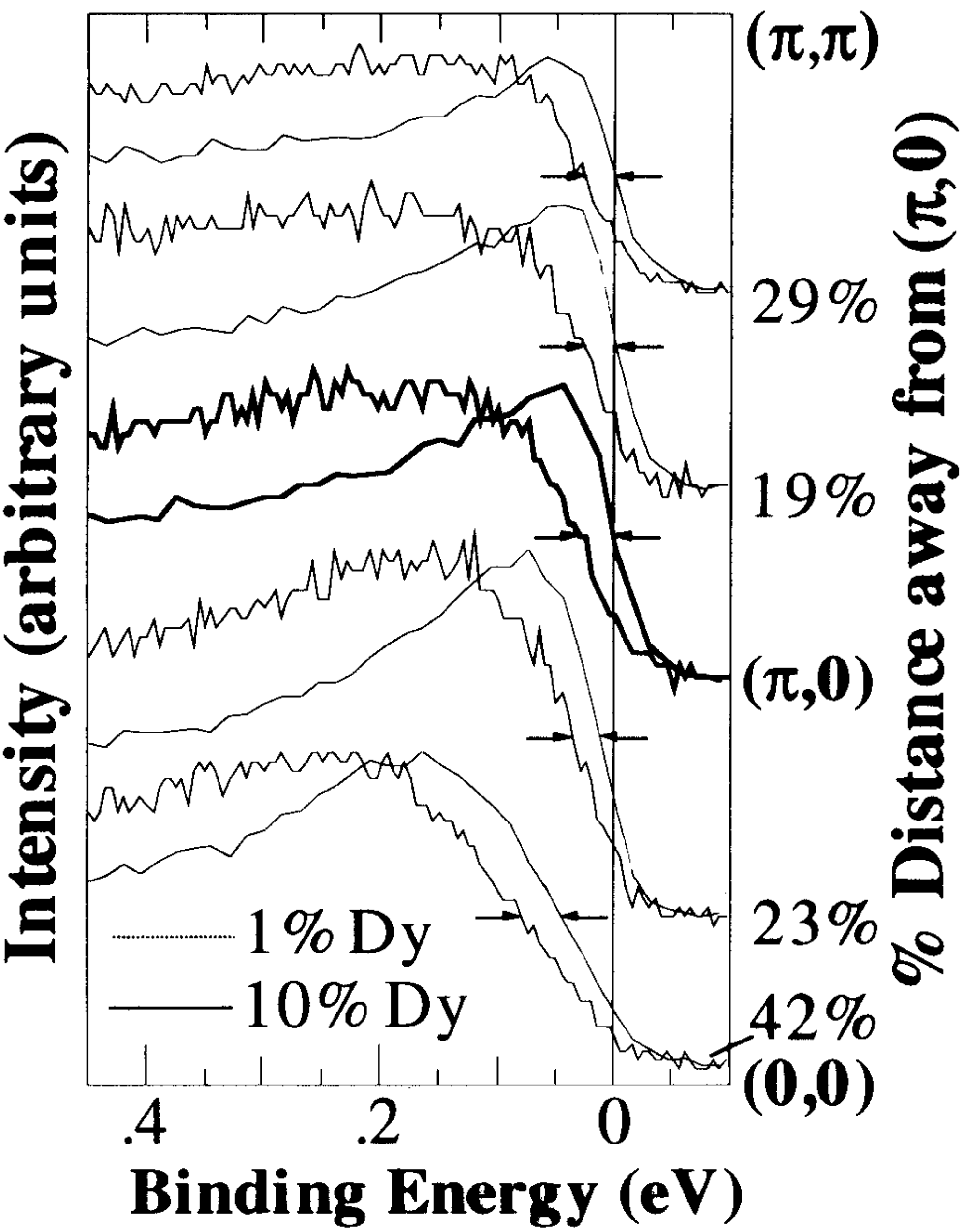

(0,0)
(π,0)
(0,π)
(π, π)



1% Dy doped Bi2212 (measured at 110K)

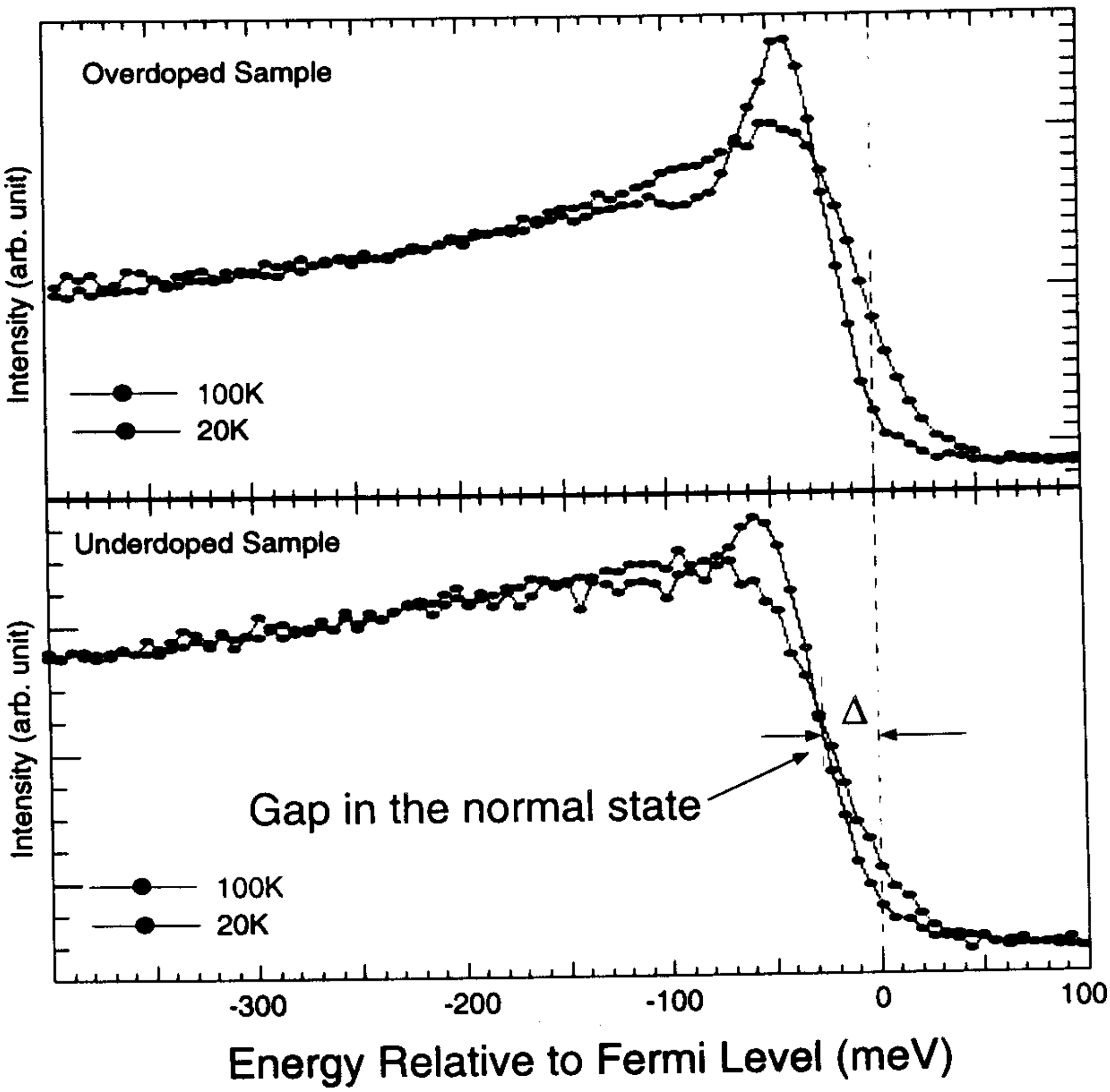


10% Dy doped Bi2212 (measured at 110K)

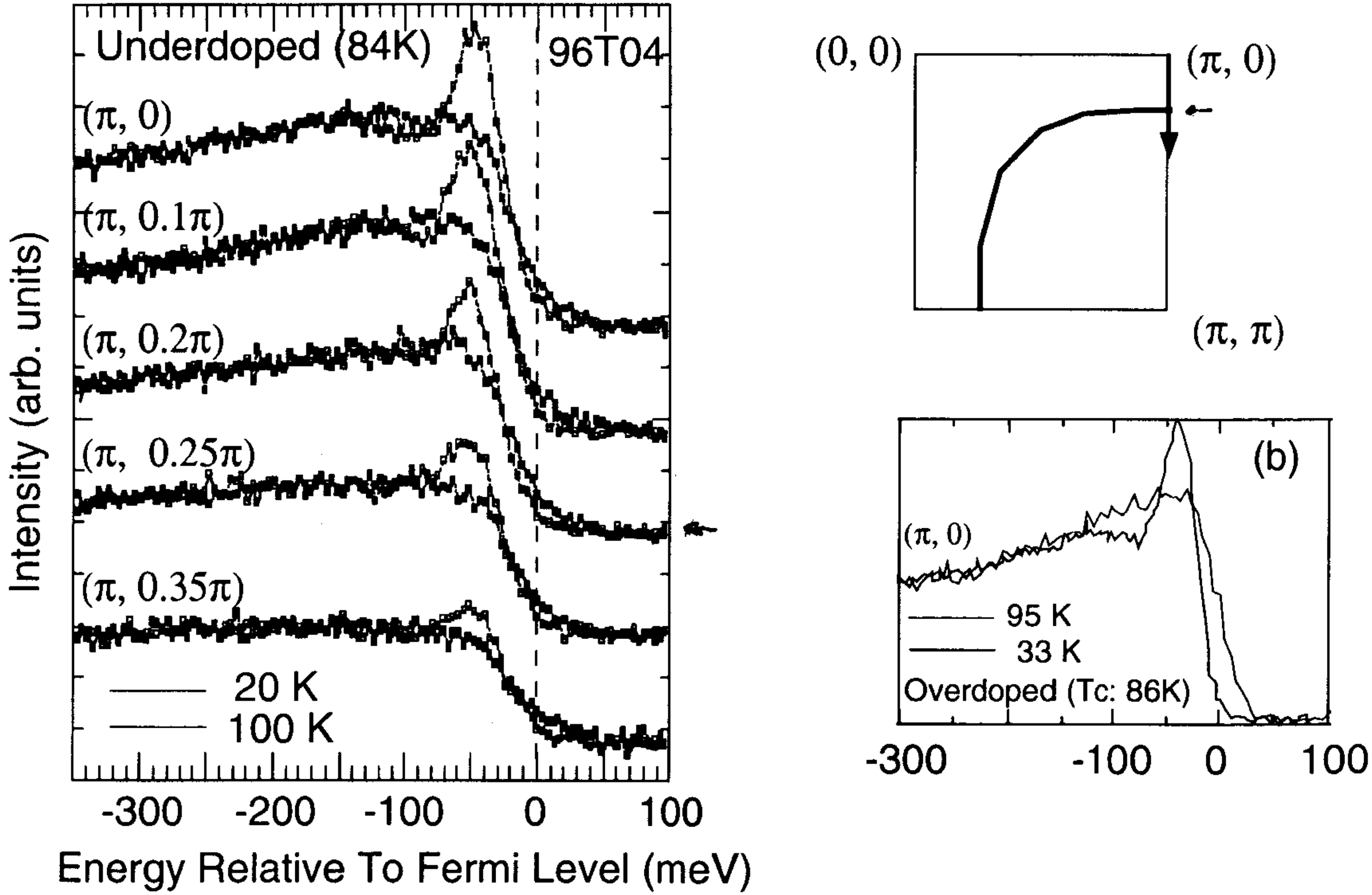


(π,π)
29%
19%
(π,0)
23%
42%
(0,0)
% Distance away from (π,0)
Intensity (arbitrary units)
1% Dy
10% Dy
.4
.2
0
Binding Energy (eV)

Observation of Pairing Gap in the Normal State



Phys. Rev. Lett. 76, 4841 (1996)
Science 273, 325 (1996)
Physics Today, June, 17 (1996)

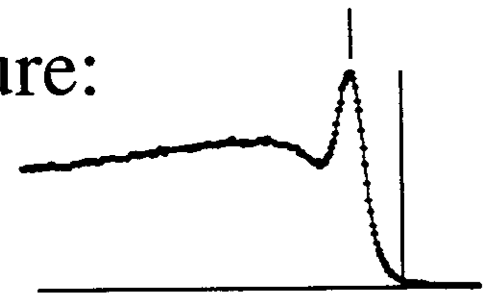


A.G. Loeser, Z.-X. Shen, et al.

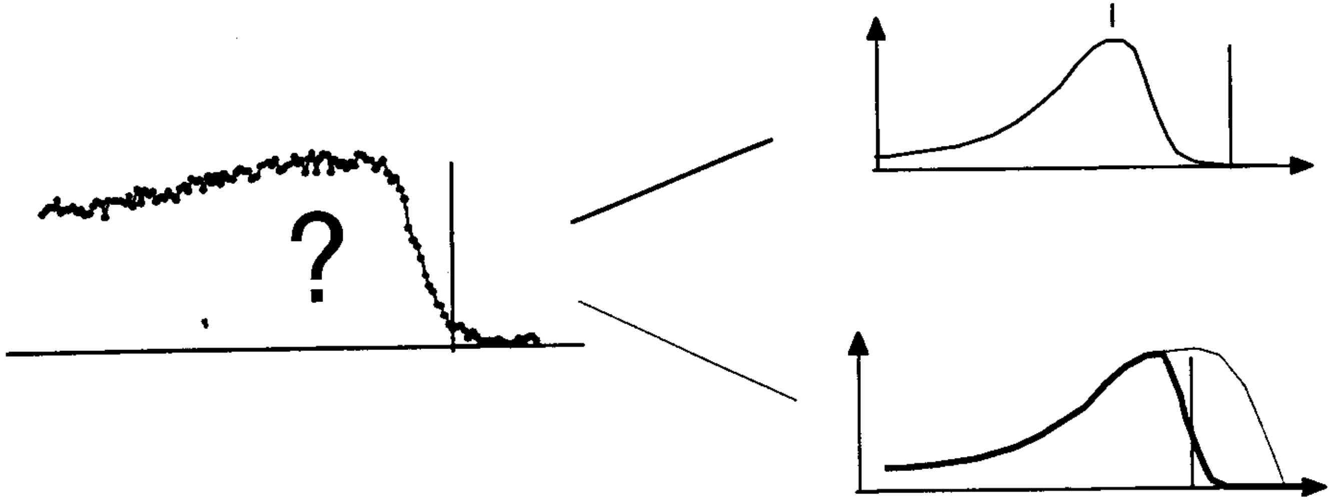
Science 273, 325 (1996)

Ways to quantify the gap

- Existence of a sharp feature:

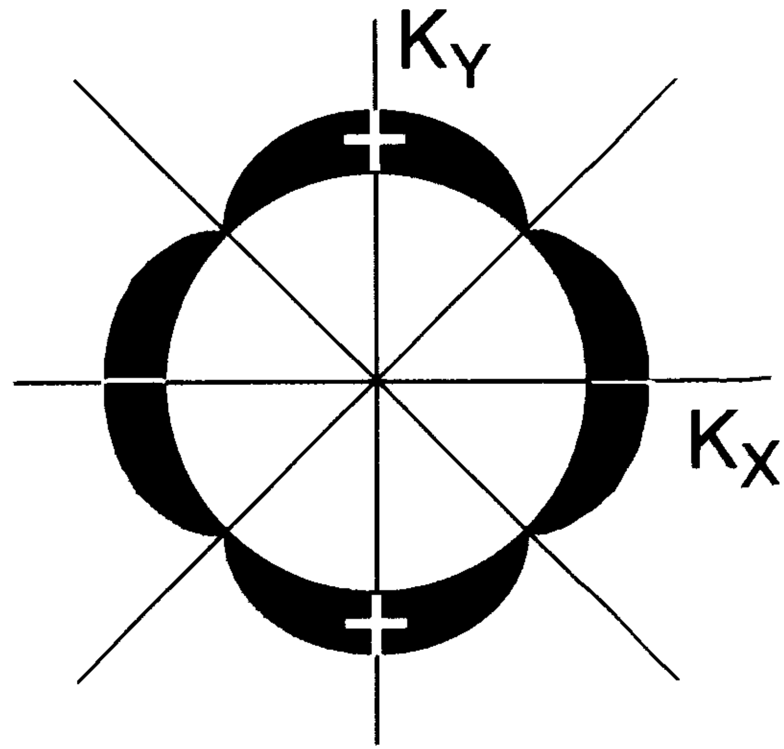


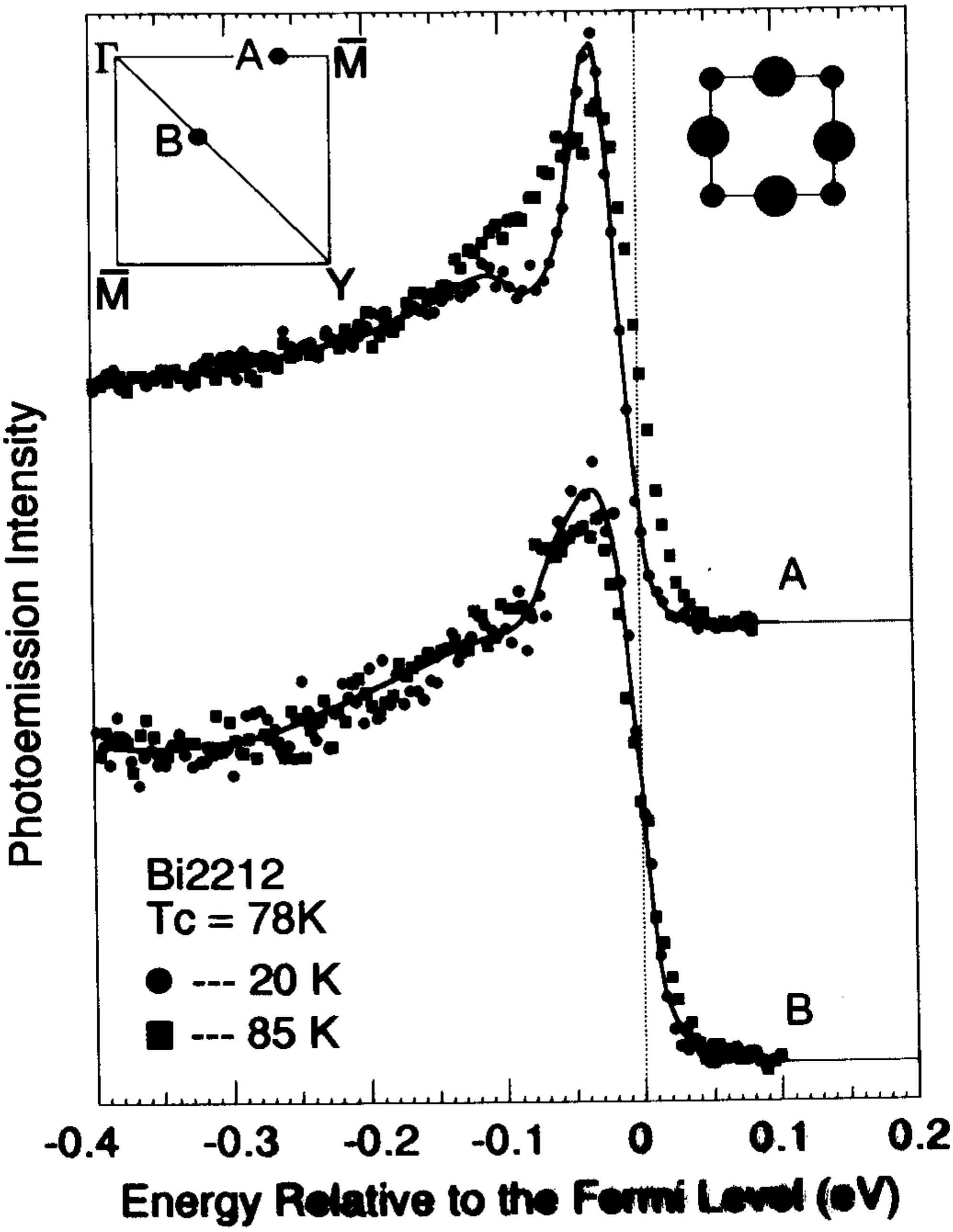
- Broad feature:



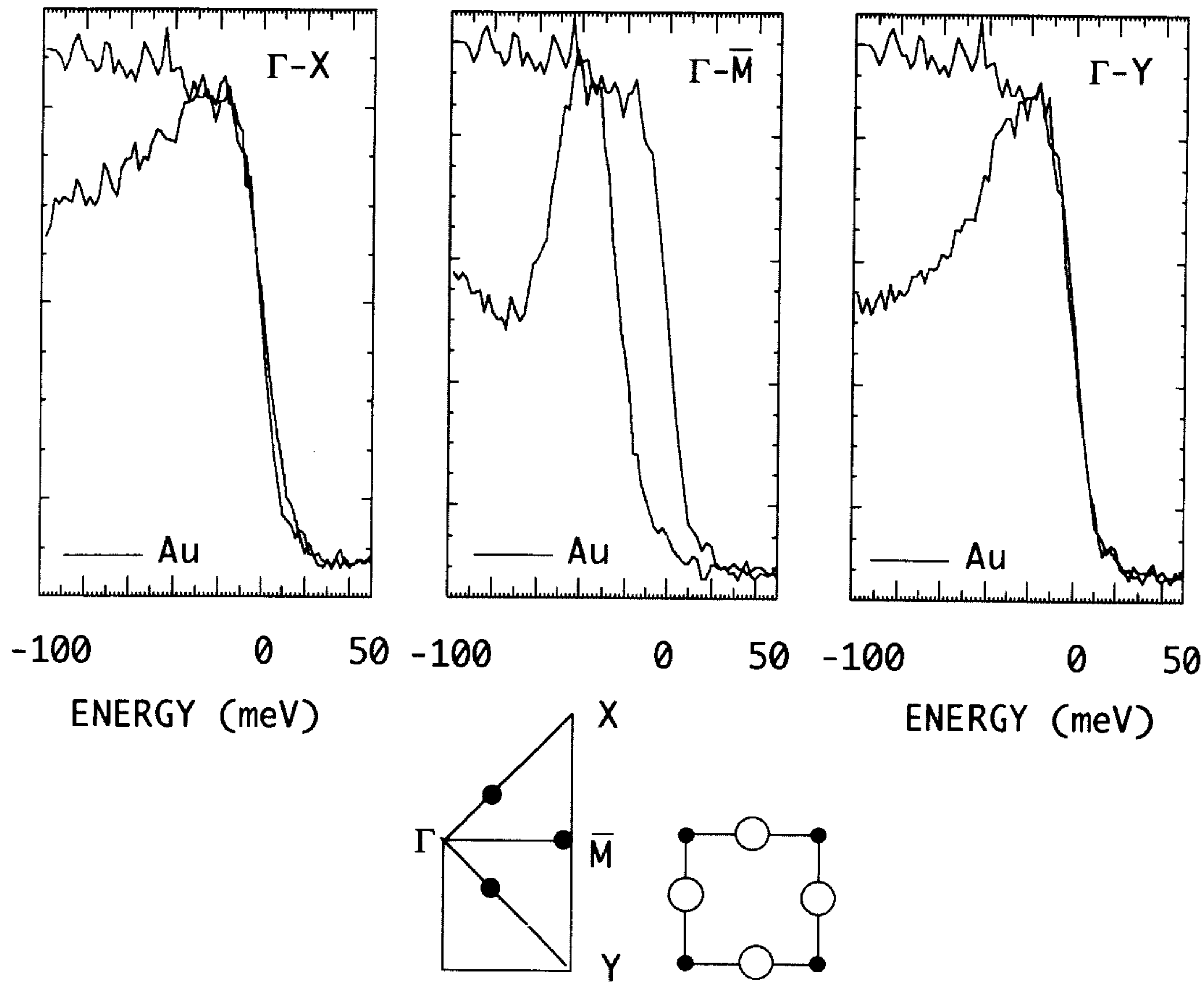
d-wave Superconductor

- Superconducting gap (minimum energy to take or add an electron) is highly anisotropic as a function of direction
- $\Delta = \Delta_0|\cos(k_x a) - \cos(k_y a)|$

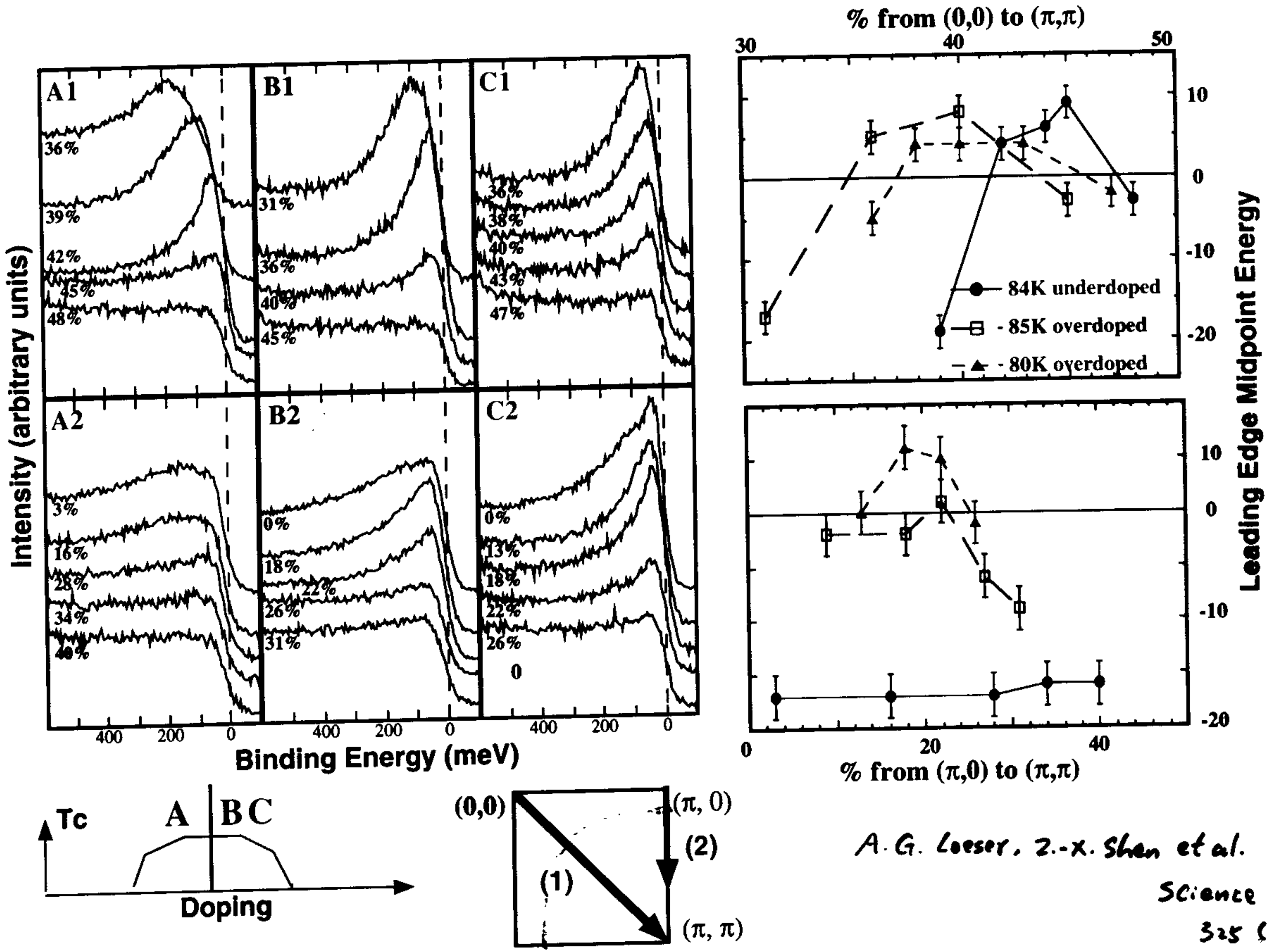




Z.-X. Shen, D.S. Dessau, B.O. Wells, et al., Phys. Rev. Lett. 70, 1553 (93)



Γ-X
Au
-100
0
50
ENERGY (meV)
Γ-M̄
Au
-100
0
50
Γ-Y
Au
-100
0
50
ENERGY (meV)
X
Γ
M̄
Y



A. G. Loeser, Z.-X. Shen et al.

Science 273
325 (1996)

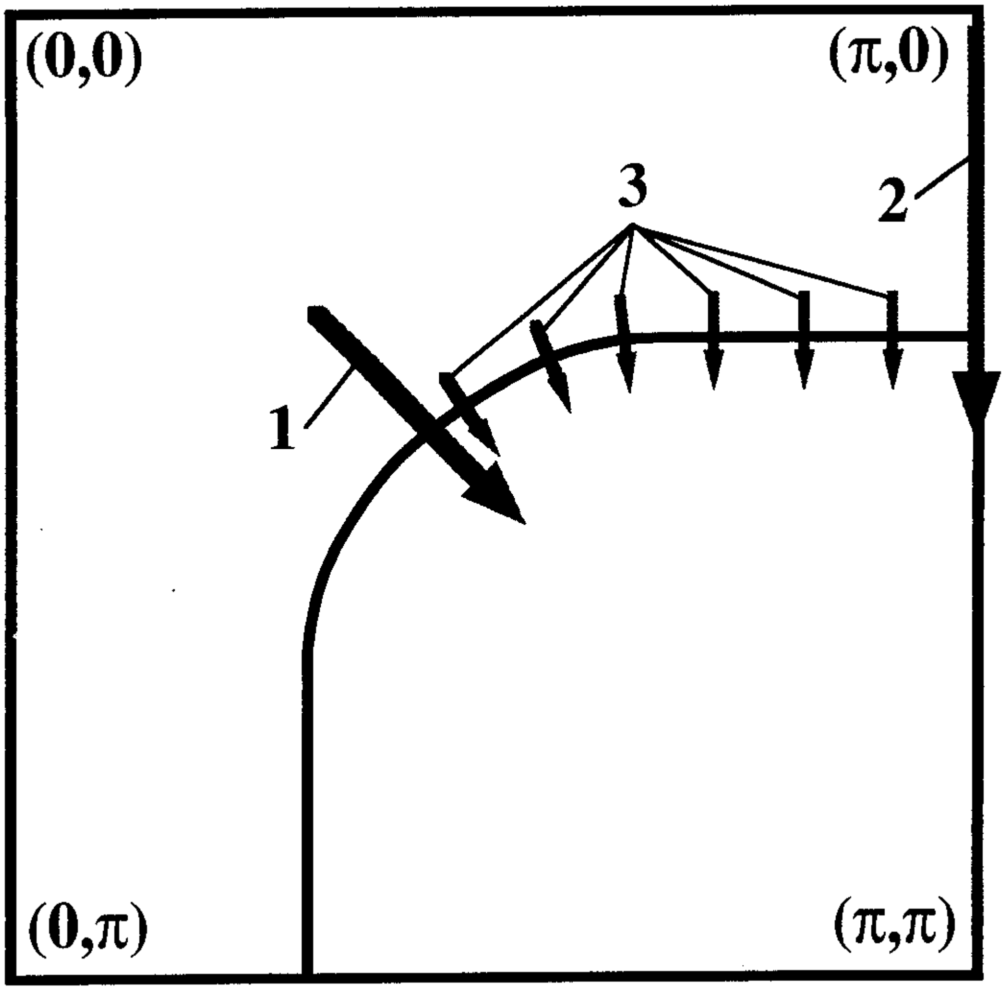
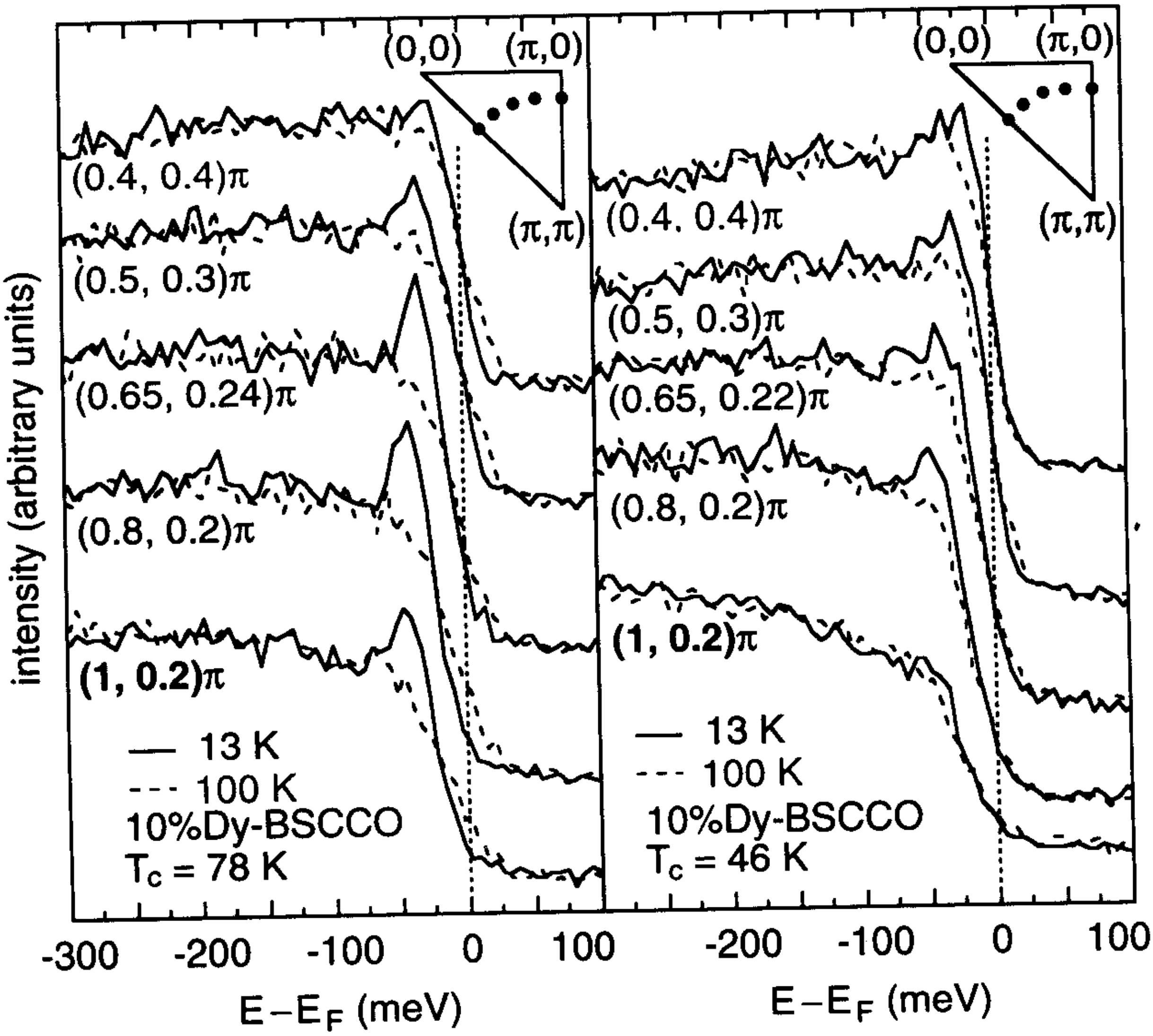


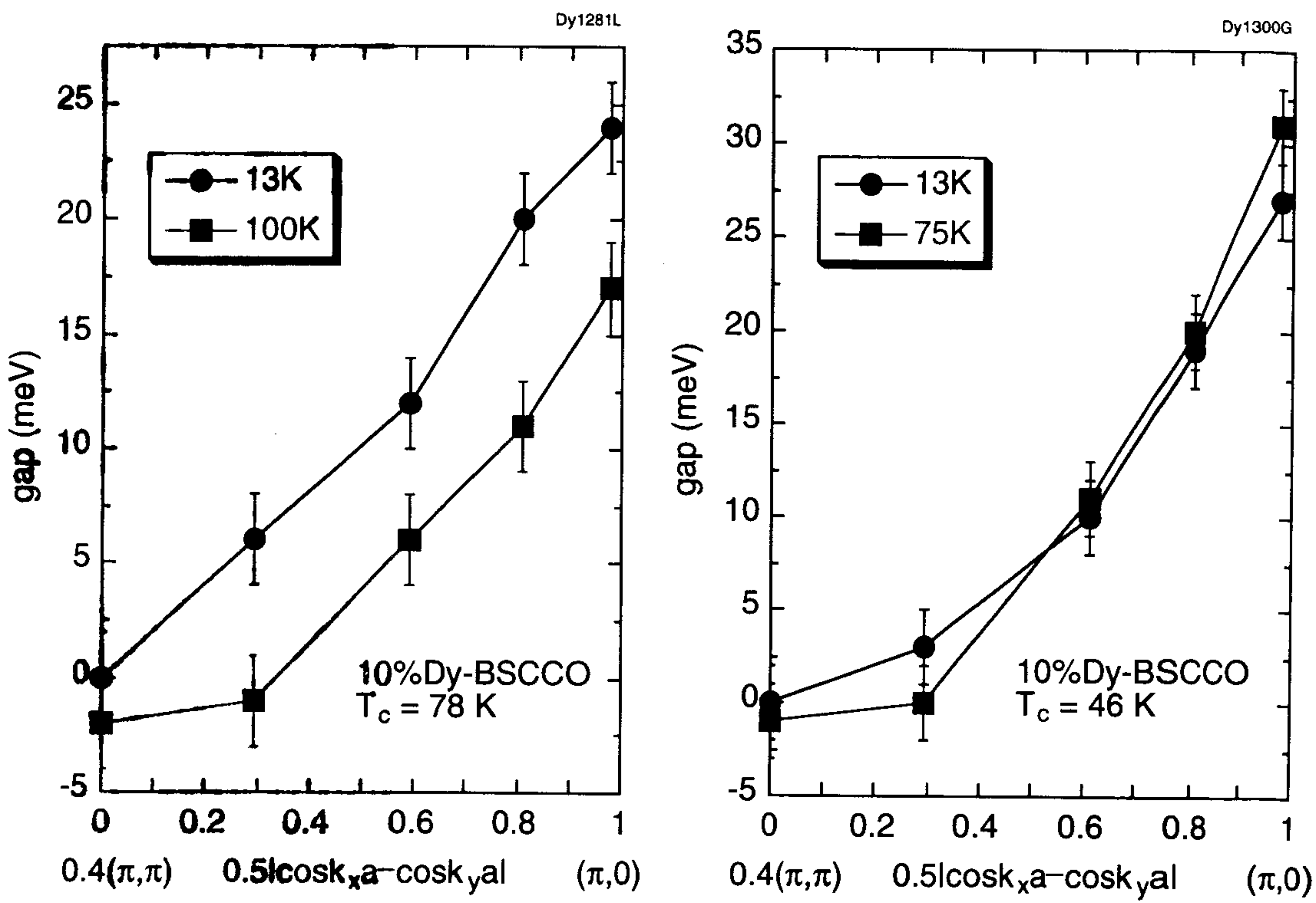
Fig2



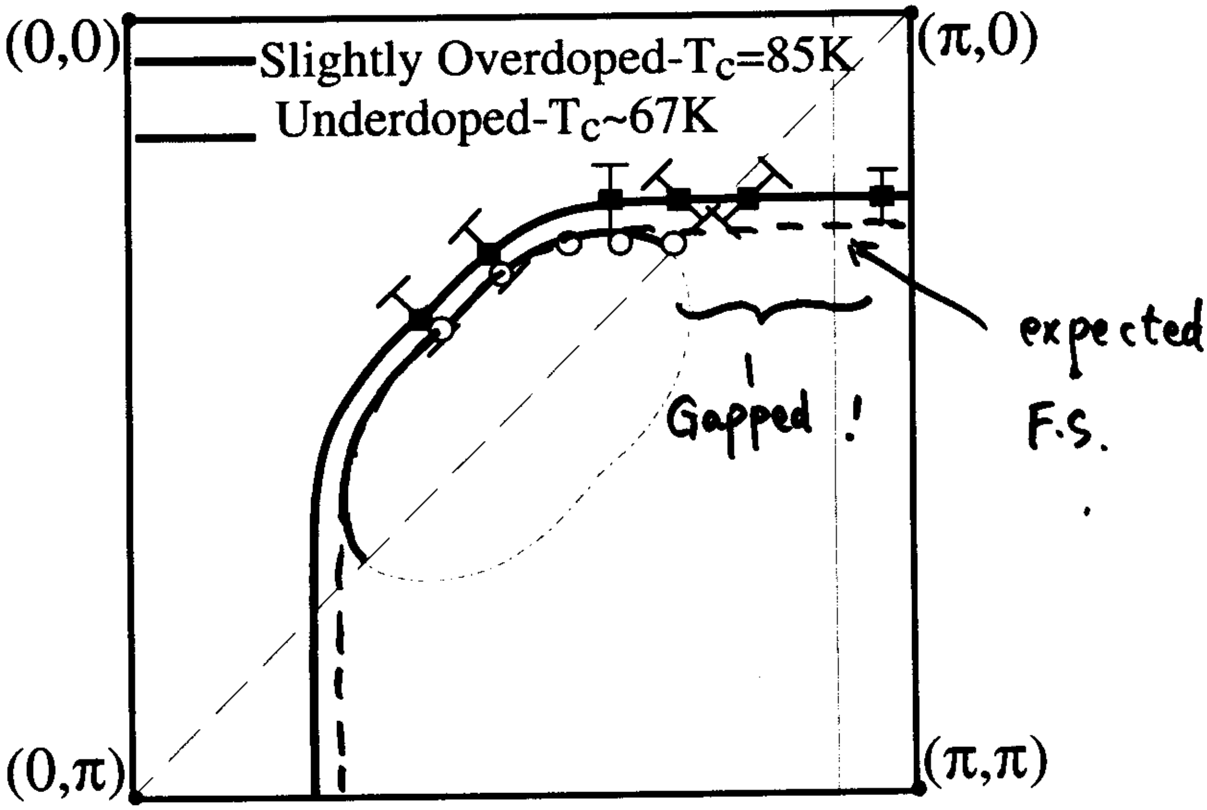
(0,0)
(π,0)
(π,π)
(0.4, 0.4)π
(0.5, 0.3)π
(0.65, 0.24)π
(0.8, 0.2)π
(1, 0.2)π
13 K
100 K
10%Dy-BSCCO
Tc = 78 K
(0.4, 0.4)π
(0.5, 0.3)π
(0.65, 0.22)π
(0.8, 0.2)π
(1, 0.2)π
13 K
100 K
10%Dy-BSCCO
Tc = 46 K
intensity (arbitrary units)
-300
-200
-100
0
100
E−EF (meV)
-200
-100
0
100
E−EF (meV)

Figure 1

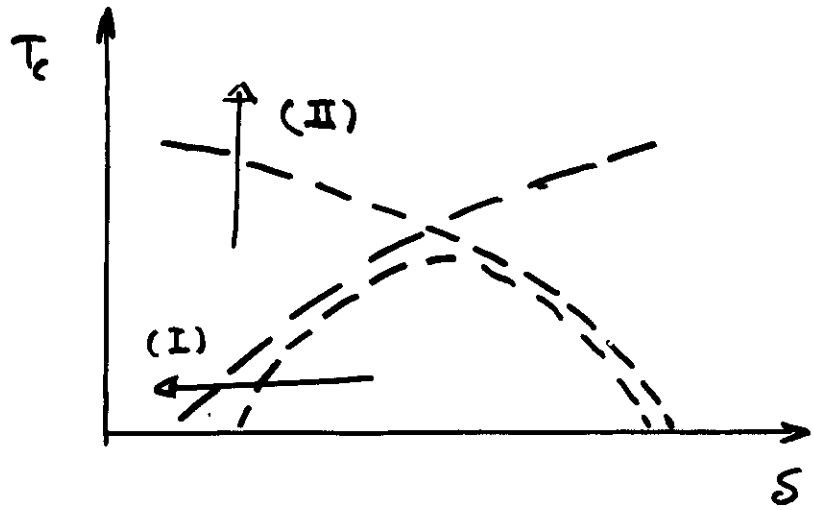
$\Delta(\vec{k})$



- Strongly anisotropic, similar to d-wave (straight line) or dirty d-wave (max |d|-c, 0) prediction
- error bars from uncertainty in Au E_F and finding leading edge midpt.



D.S. Marshall et. al., PRL 76, 4841 (1996)



I. Superconducting Gap vs. doping

II. Normal State Gap vs. Temperature

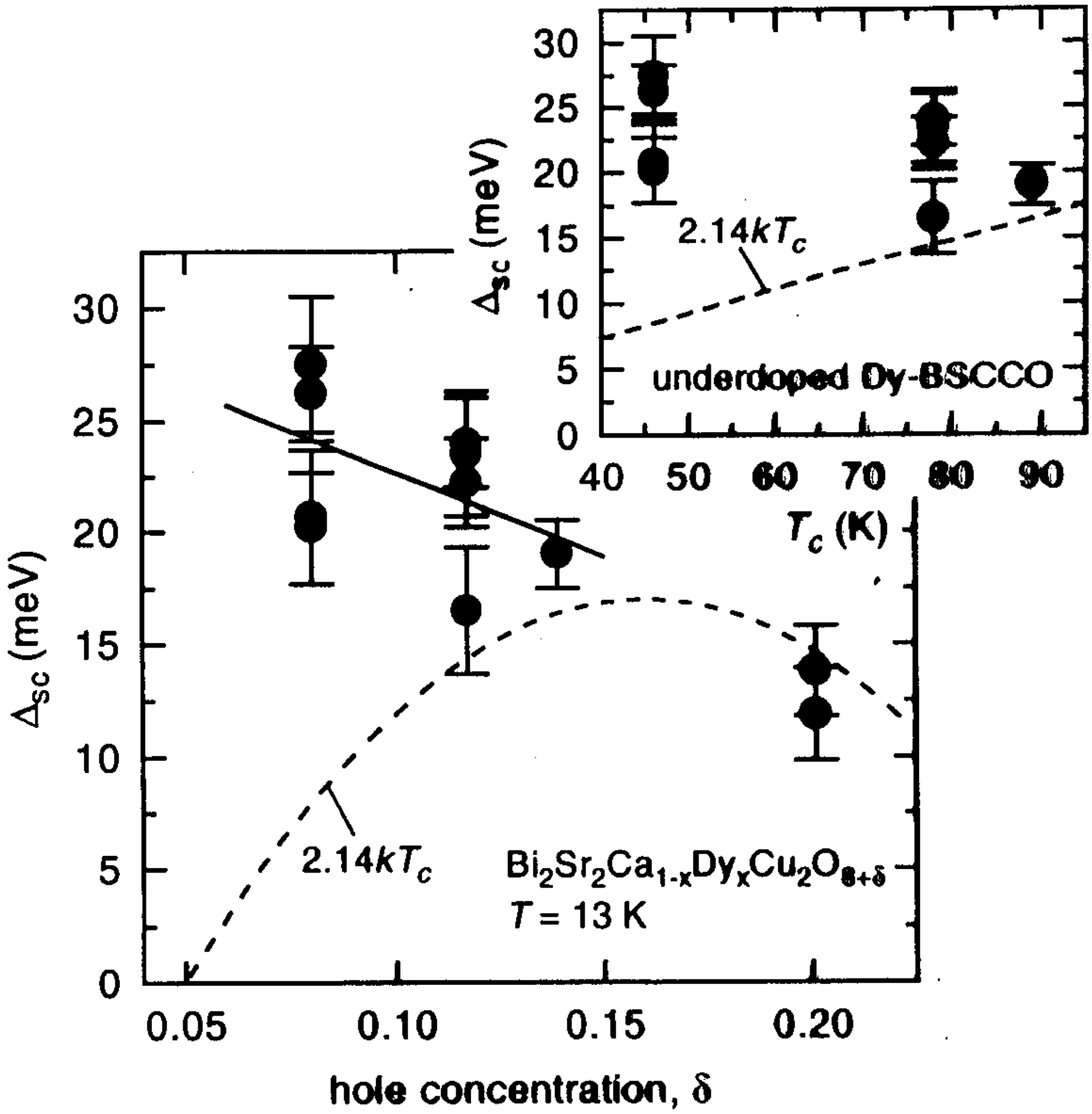
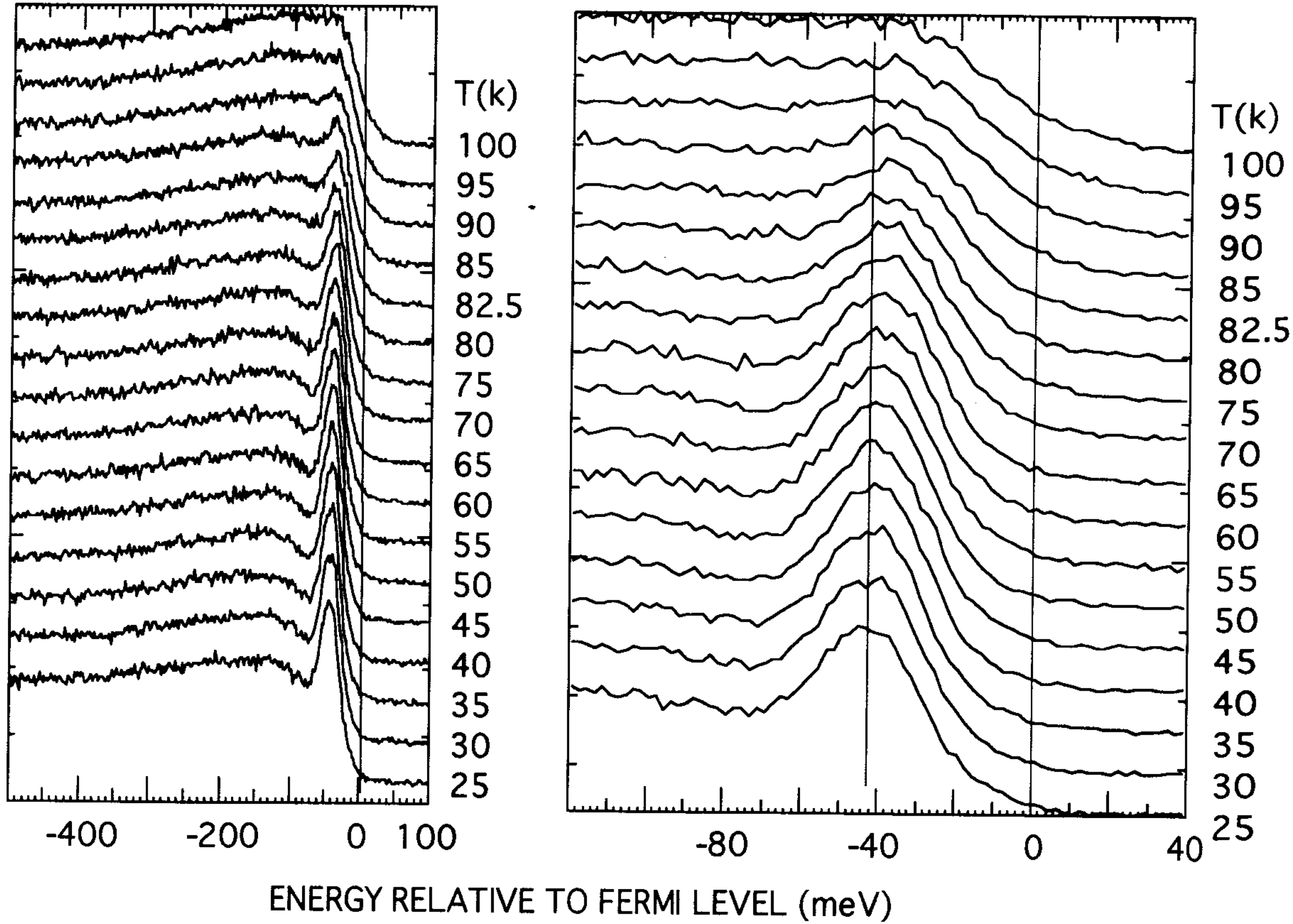
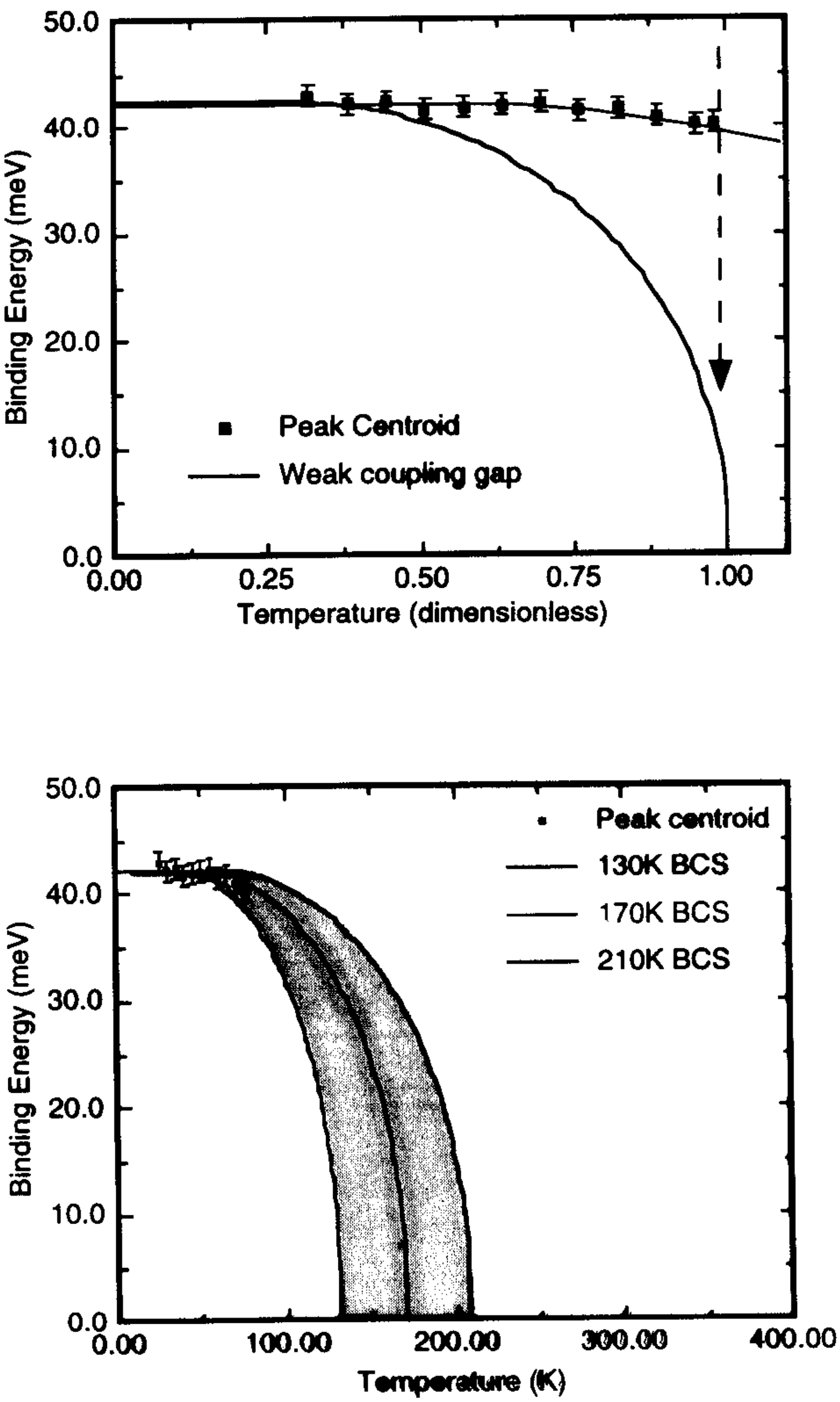


Figure 4

J. M. Harris et al., PRB 54, R15665 (1996)

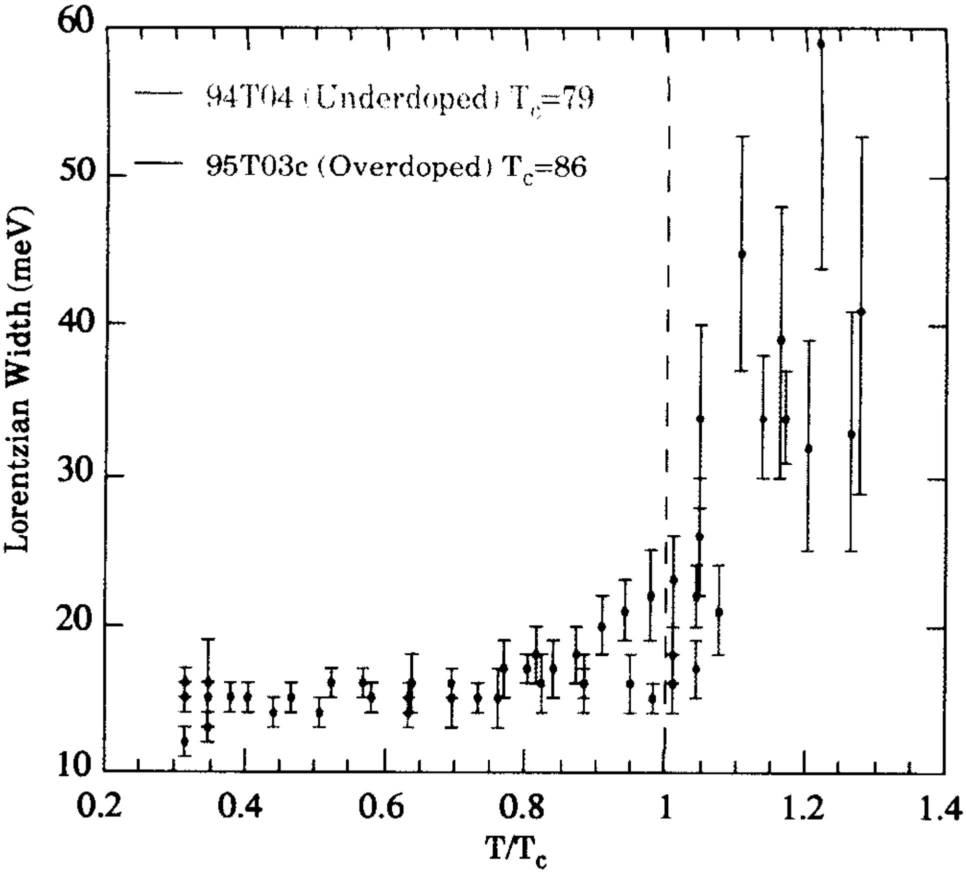
Temperature Dependent Spectra at Mbar (Sample 94T04)



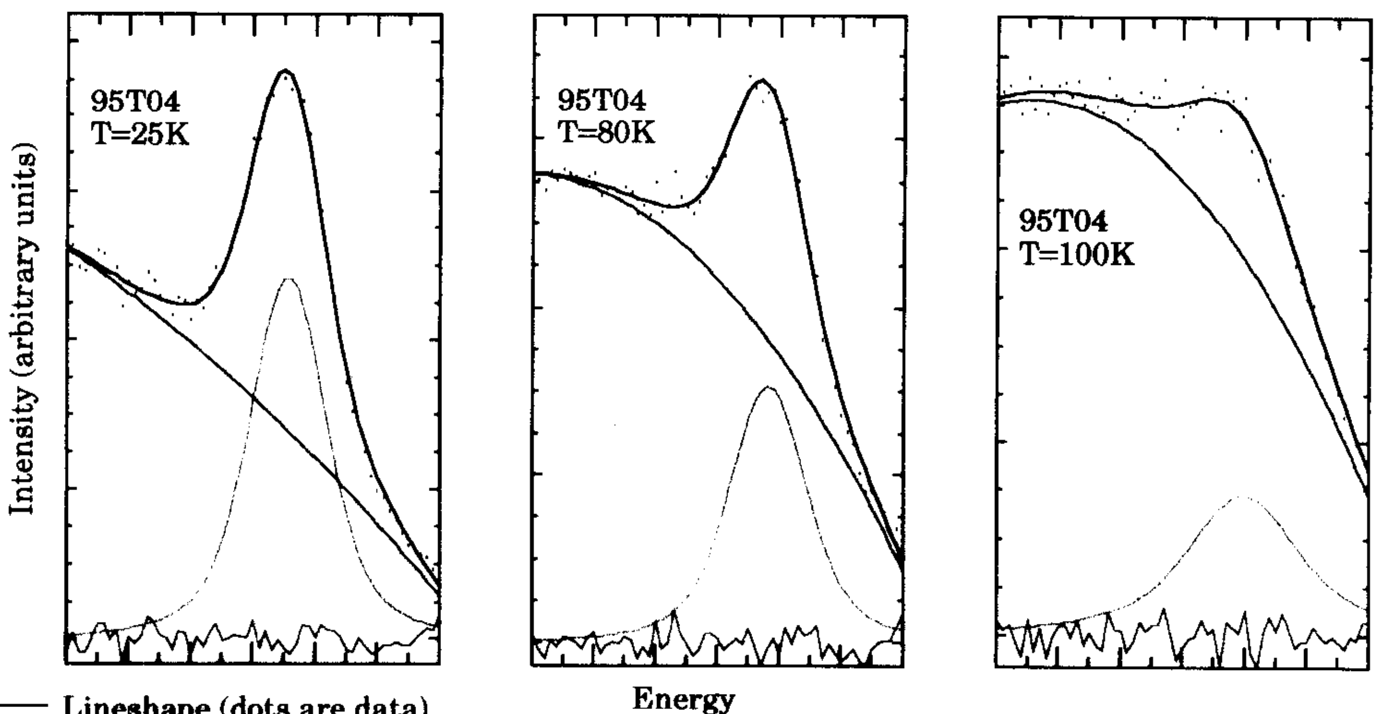


Bi2212 : underdoped, Tc = 79K

Width of sharp feature at $\overline{M}$



- Below T_c, fits are robust.
- At low temperatures, the FWHM is fairly constant.
- Above T_c, the width increases drastically.
- Above T_c, "background" lineshape may be misleading, and fits are less convincing.



Lineshape (dots are data)
Background
Fitted peak
Residual

Sample fits of sharp feature

- Energy window 120meV
- Instrumnt broadening 20meV
- Background 2nd order poly.

Peak Width Chart

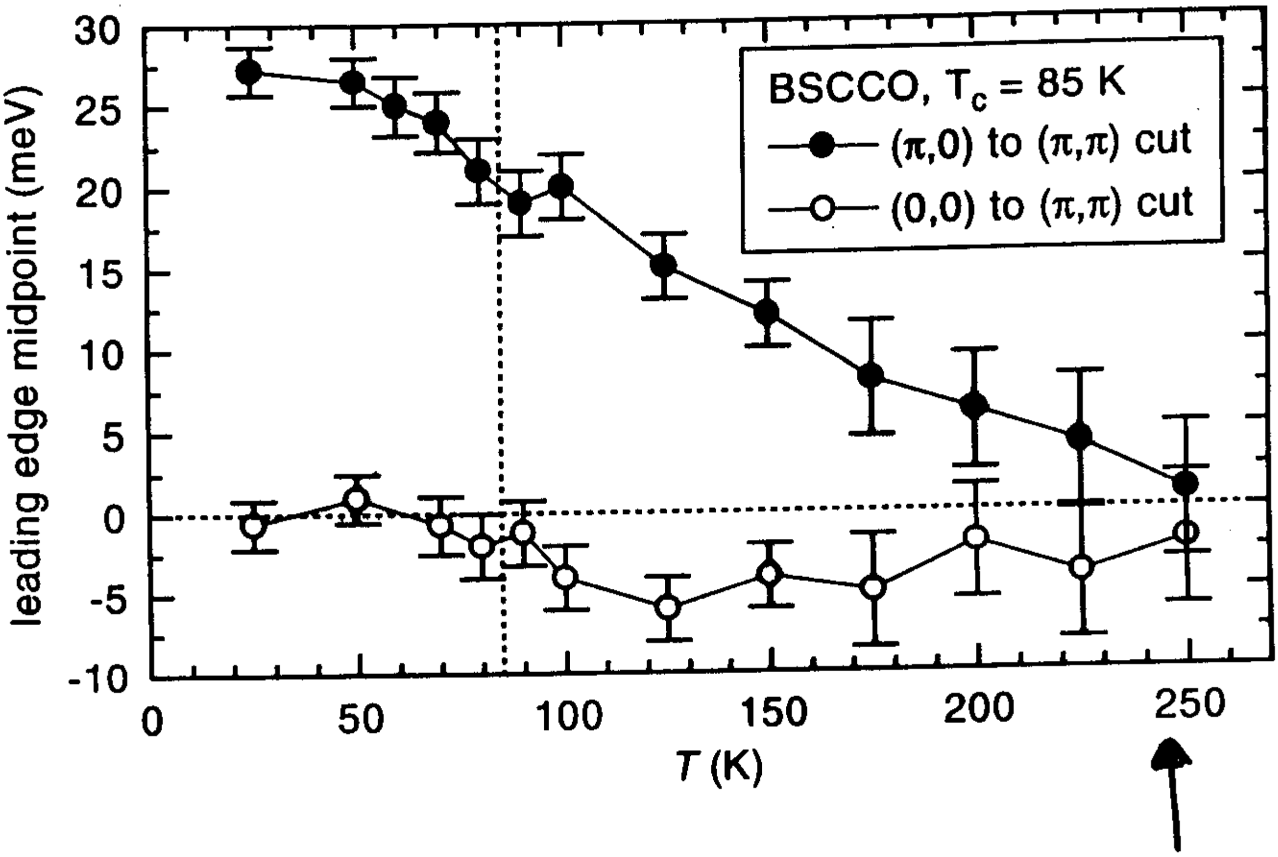
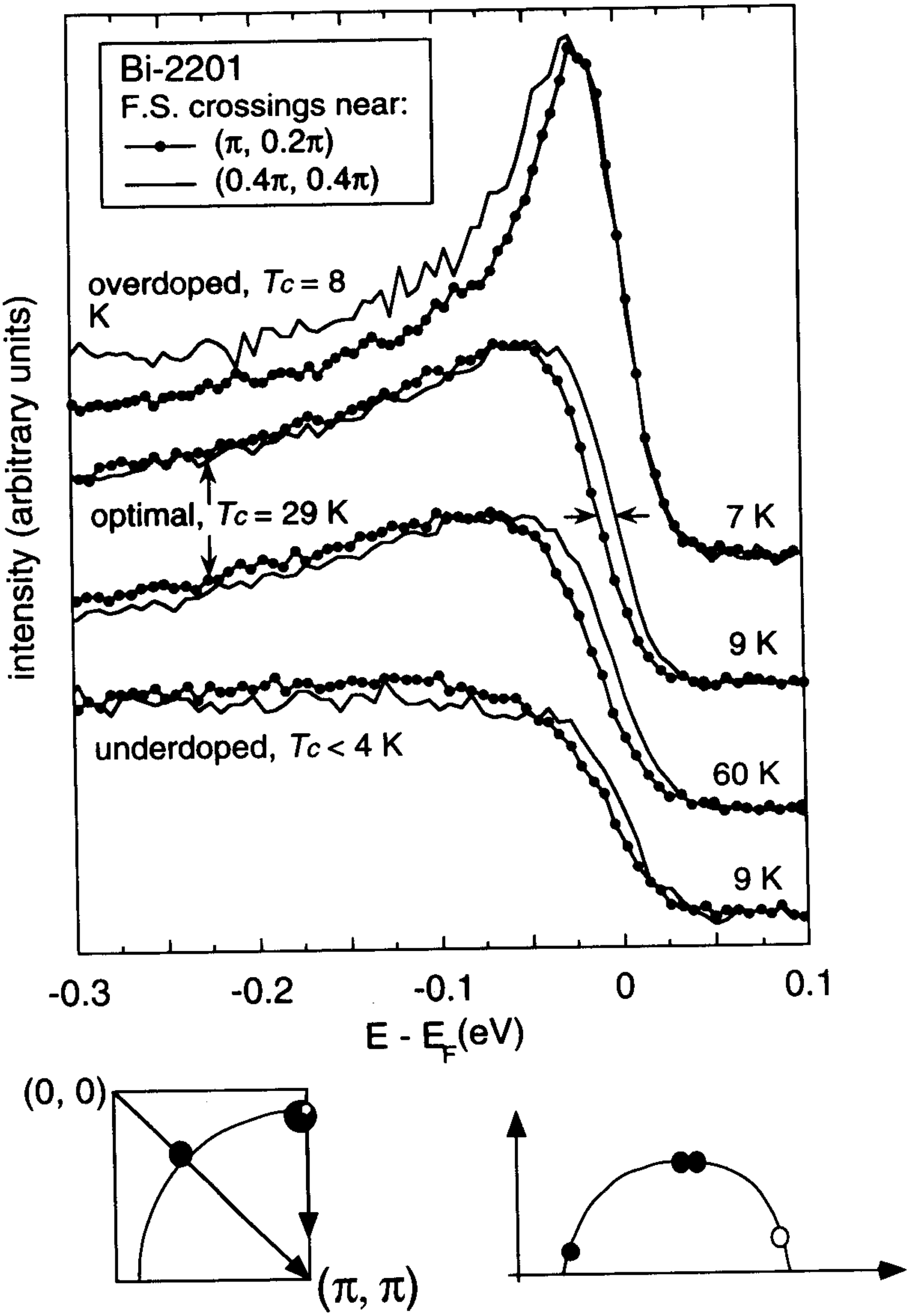


Figure 3

J. M. Harris et al., PRB 54, R15665 (1996)

Summary

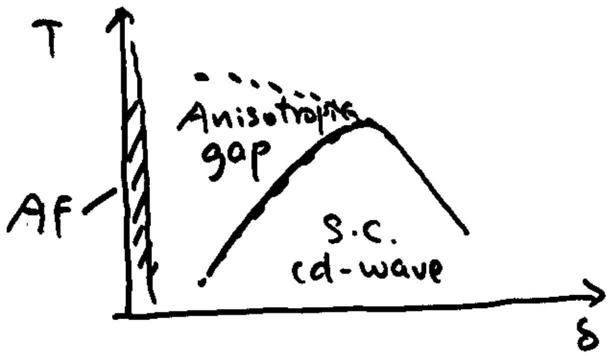
- Anomalous Properties of Bi2212
  - Excitation Gap in the Normal State of "Underdoped" Bi2212
  - Normal State Gap is Very Similar to the dx2-y2 Superconducting Gap
  - The Superconducting Gap Does Not Decrease with Tc in Underdoped Regime
  - The Superconducting Gap Decreases with Tc in Overdoped Regime
  - There Is a Higher Temperature Scale > Tc



Bi-2201
F.S. crossings near:
(π, 0.2π)
(0.4π, 0.4π)
overdoped, Tc = 8 K
optimal, Tc = 29 K
underdoped, Tc < 4 K
7 K
9 K
60 K
9 K
intensity (arbitrary units)
-0.3
-0.2
-0.1
0
0.1
E - EF(eV)
(0, 0)
(π, π)

Summary:

* Bi2212 & Bi2201 have a similar phase diagram



Anisotropic gap ⟷ S.C. gap

Different from pseudogap in Mn oxides.

* $$\frac{\Delta(2212)}{\Delta(2201)} \sim \frac{T_{c\,max}(2212)}{T_{c\,max}(2201)} \ ?$$