Polaronic Effects in the Lightly Doped Cuprates

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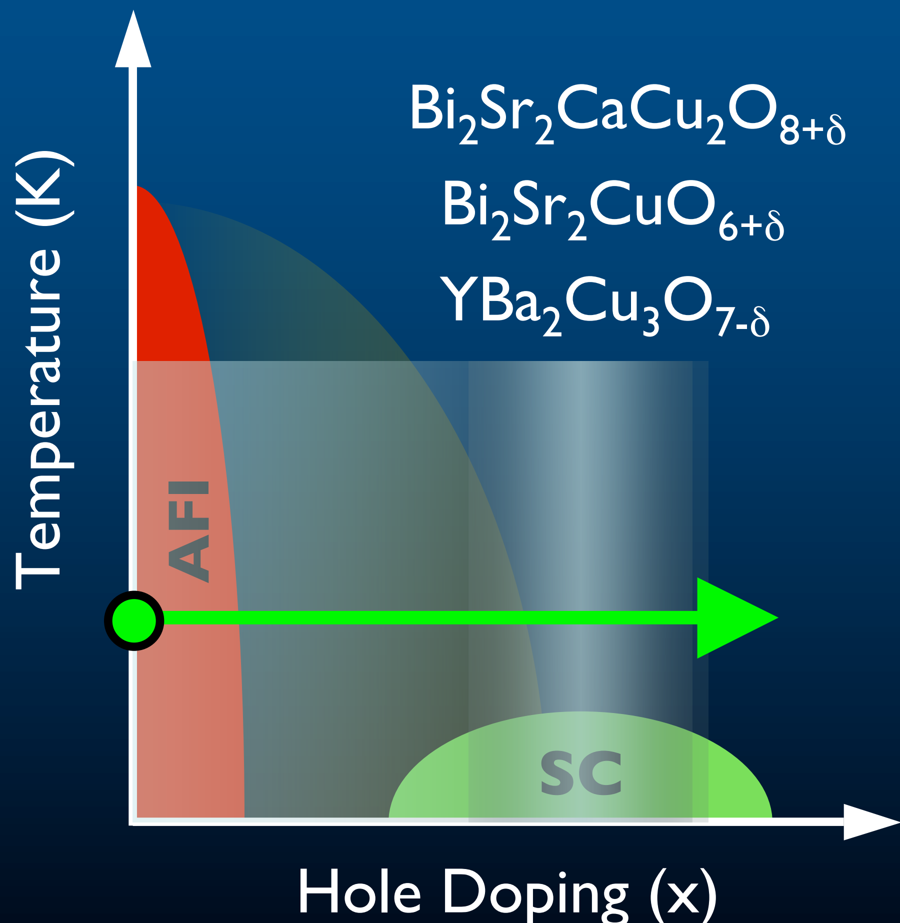
Stanford University

April 6, 2005

ARPES Studies of the Cuprates



Physics of *"Lightly Doped"* Mott Insulators?

"High-Temperature Superconductivity is the physics of strong correlations"

Phase Diagram of $Ca_{2-x}Na_xCuO_2Cl_2$

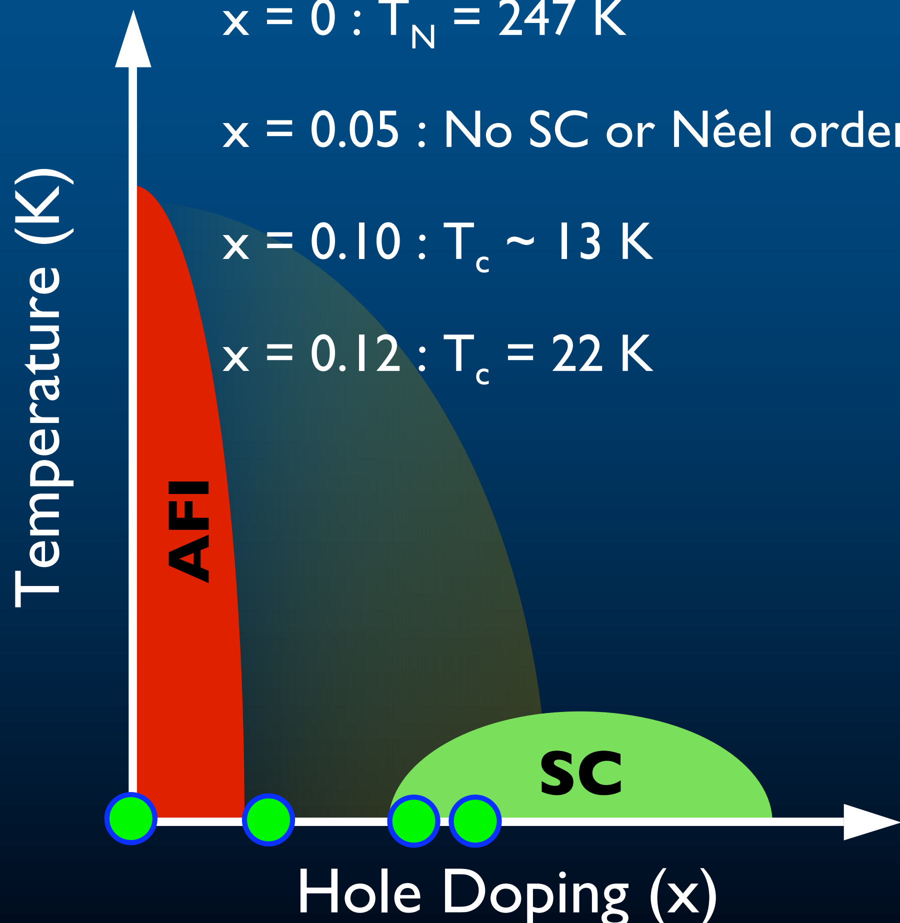
$T_{c,max}$ = 28 K @ x = 0.18

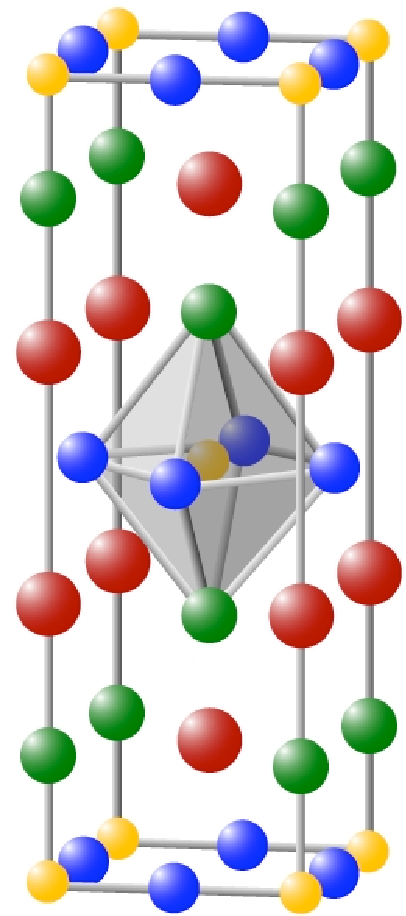
x = 0 : T_N = 247 K

x = 0.05 : No SC or Néel order

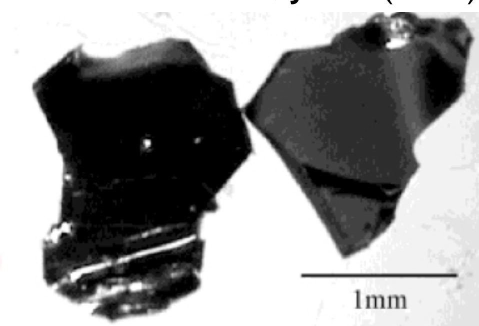
x = 0.10 : T_c ~ 13 K

x = 0.12 : T_c = 22 K





Y. Kohsaka *et al.*, JACS (2002)

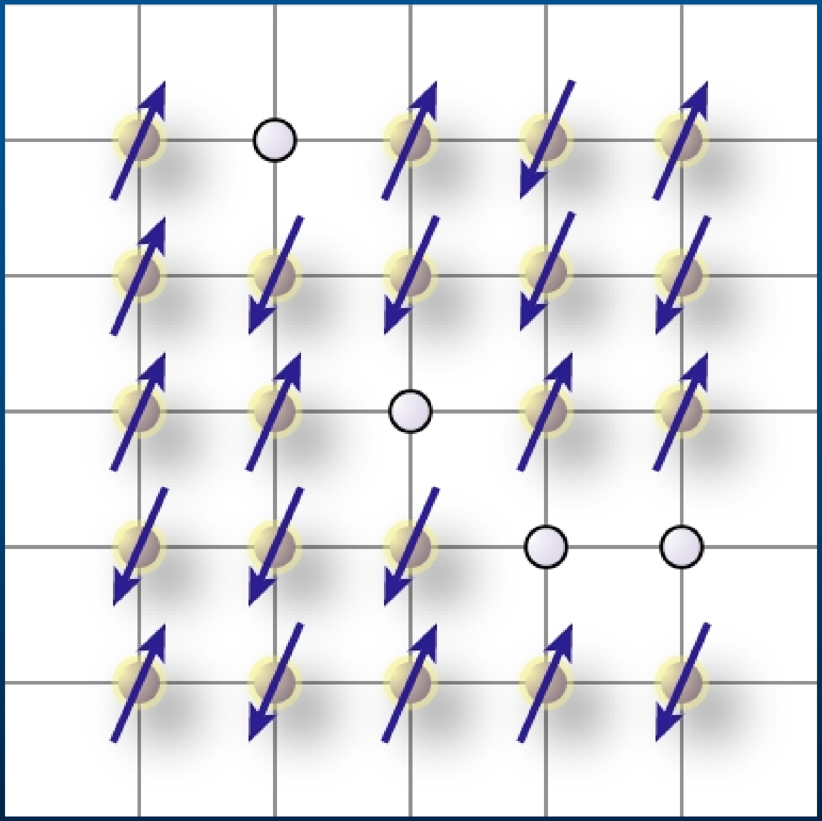


Tetragonal K_2NiF_4 Structure

Undistorted square CuO_2 planes

Grown under high pressures (~ 4 GPa)

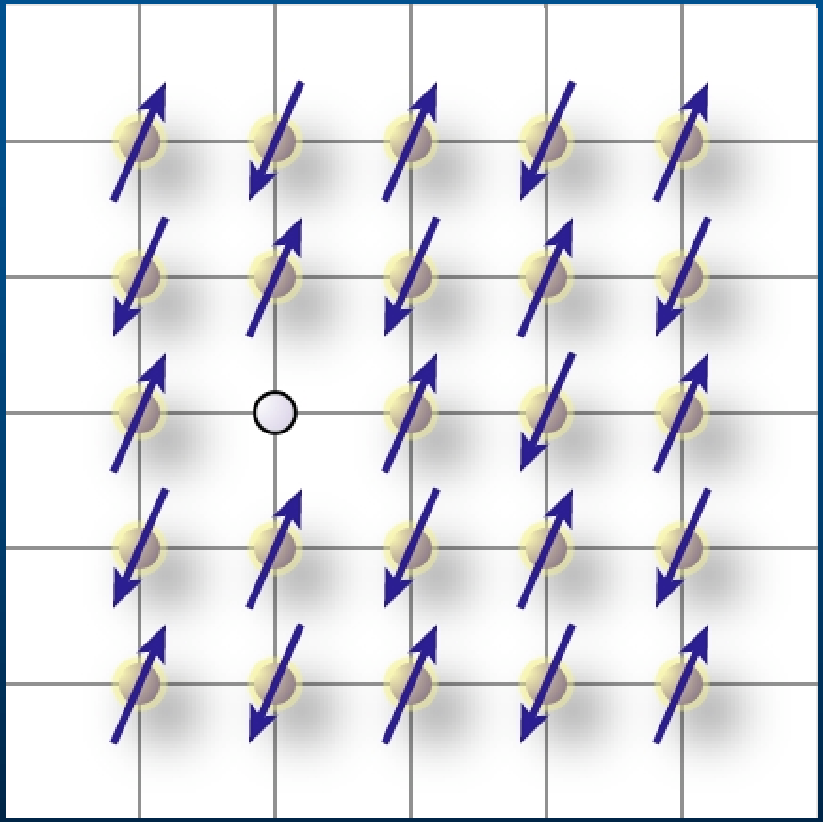
Many-Body Interactions in Cuprates



Studying interactions of many holes with spin, lattice, charge degrees of freedom an intractable theoretical problem...

Can we simplify the problem (both experimentally and theoretically?)

A Single Hole in the Mott Insulator

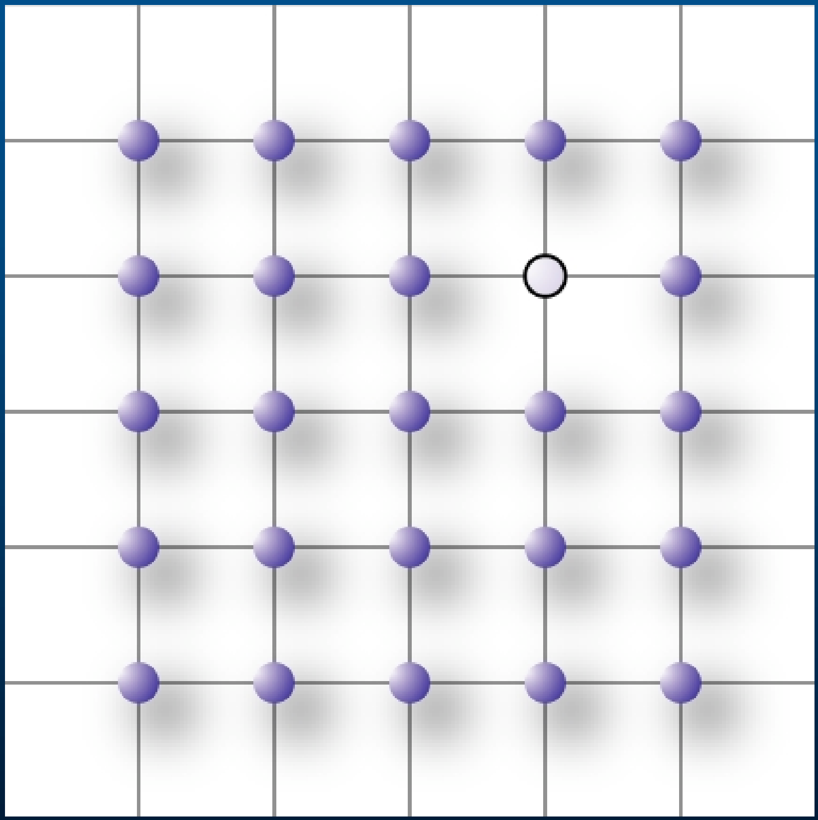


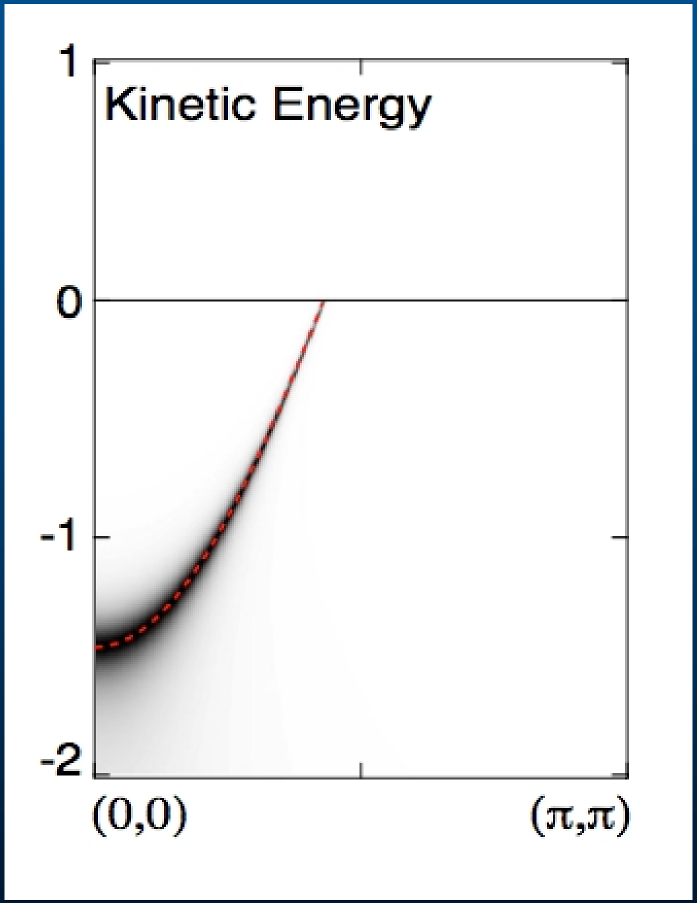
ARPES on Mott insulator : Reflects dynamics of *a single hole*!

A logical starting point for understanding relevant interactions

Band Structure Predictions : Non-Interacting

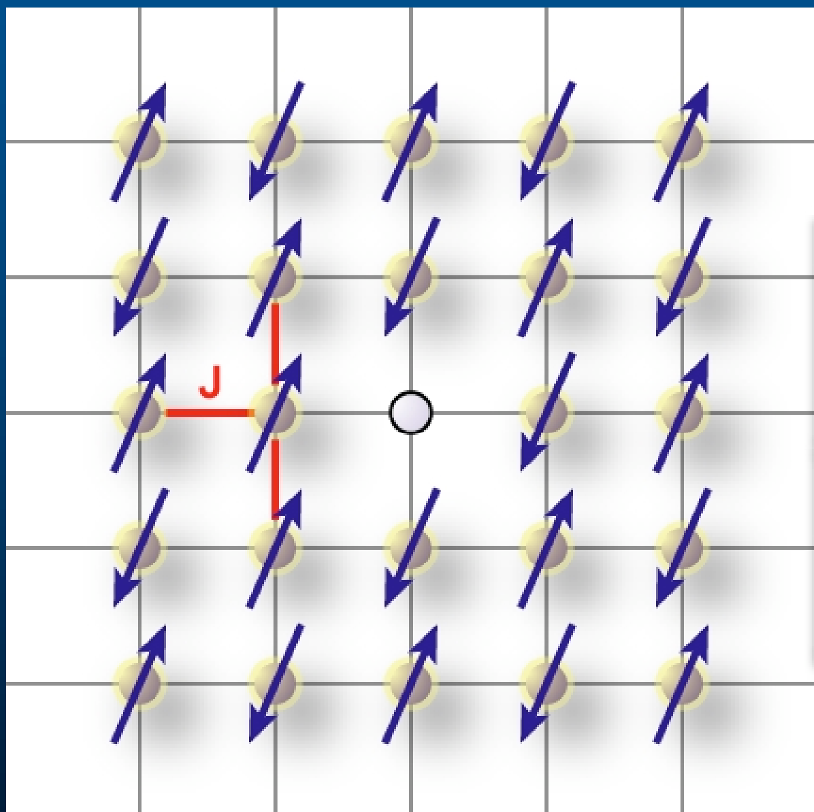
Kinetic Energy Only

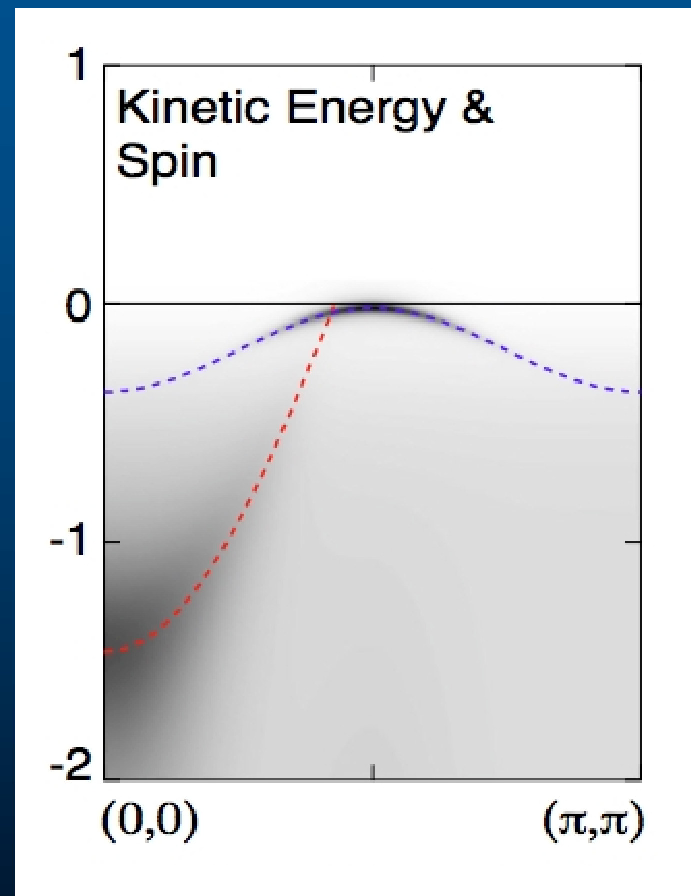




Mott Insulator : Magnetic Interactions

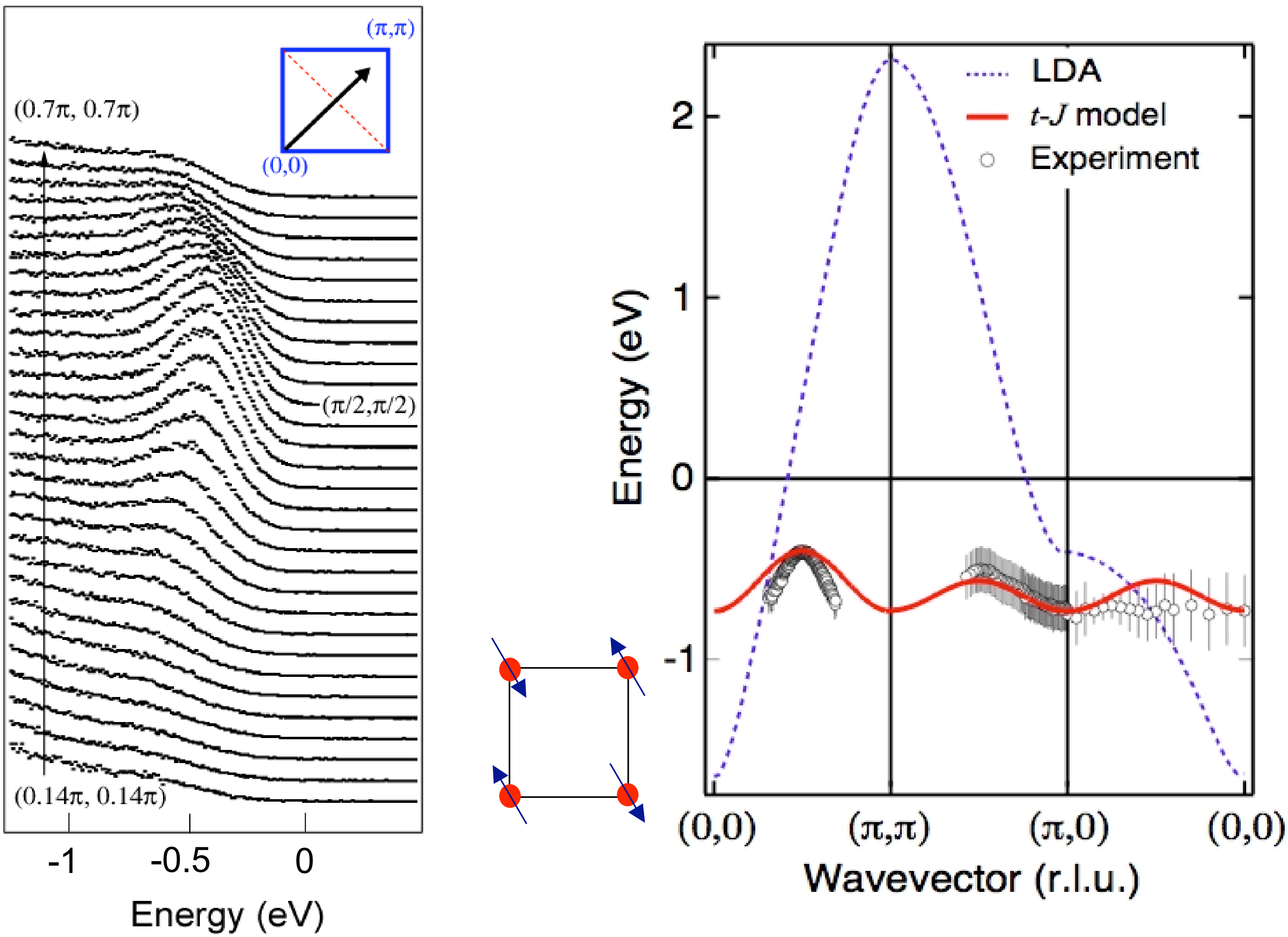
KE & Magnetism





t-J :
$$\mathcal{H} = -t \sum_{\langle ij \rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle,\sigma} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4})$$

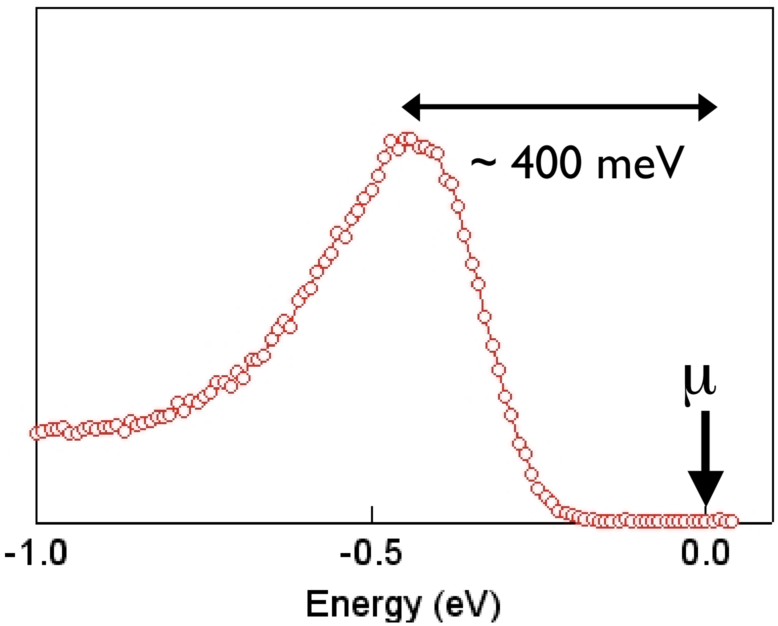
A Single Hole in the Mott Insulator



Comparison with Fermi Liquid

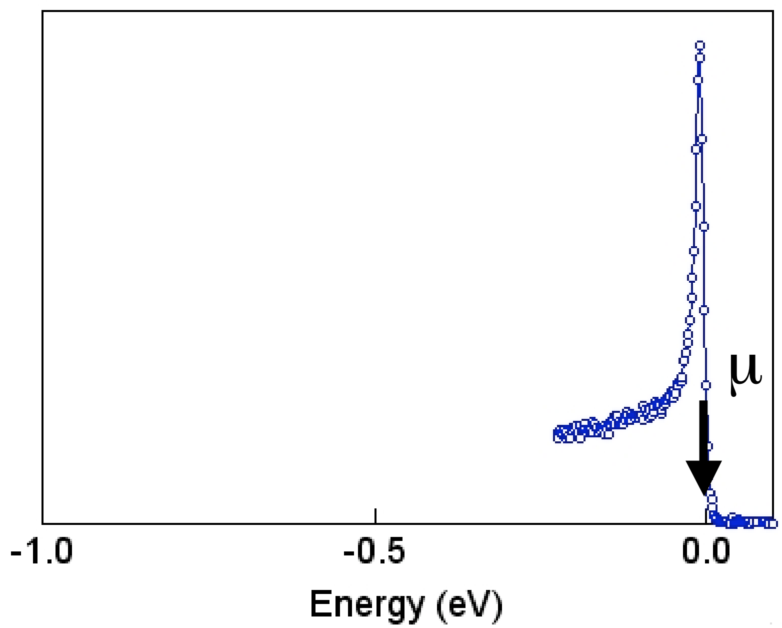
$Ca_2CuO_2Cl_2$

1. Peak Width ~ 300 meV
2. Gaussian Lineshape
3. Separation of μ from peak



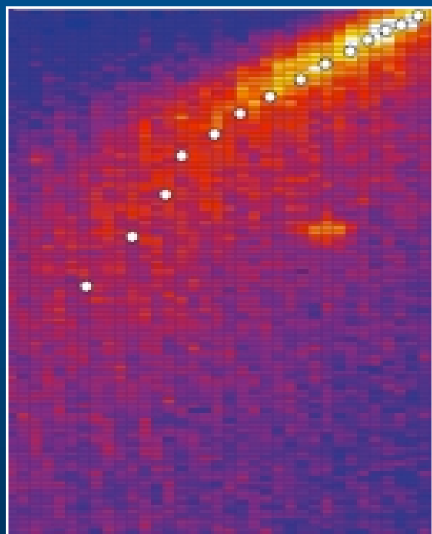
Sr_2RuO_4

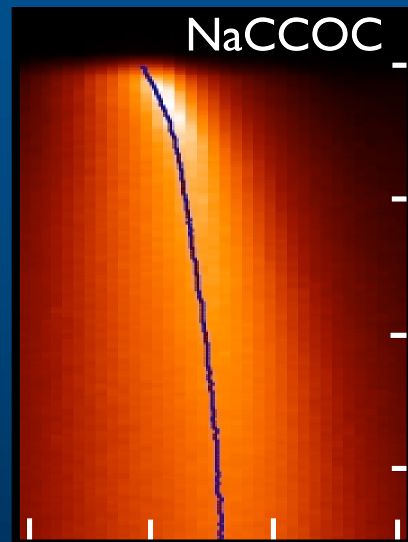
1. Peak Width ~ 10 meV
2. Lorentzian (FL) Lineshape
3. Peak approaches μ

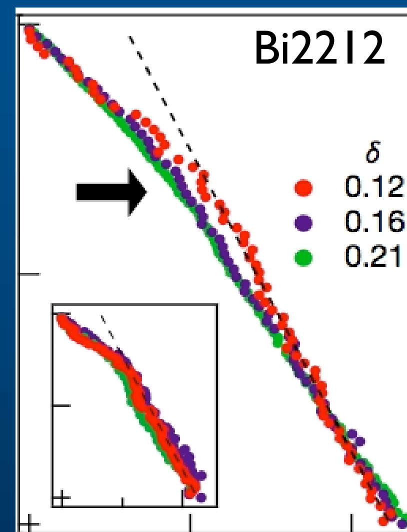


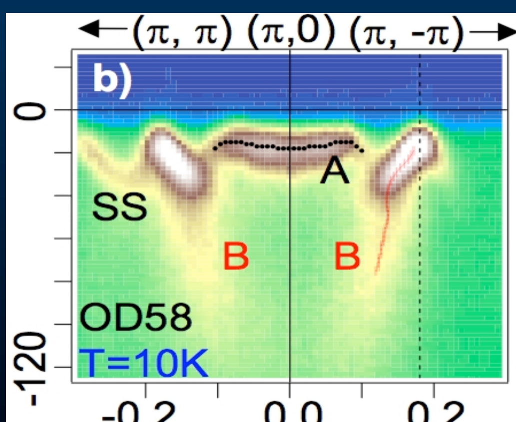
Electron-Boson Interactions in Cuprates

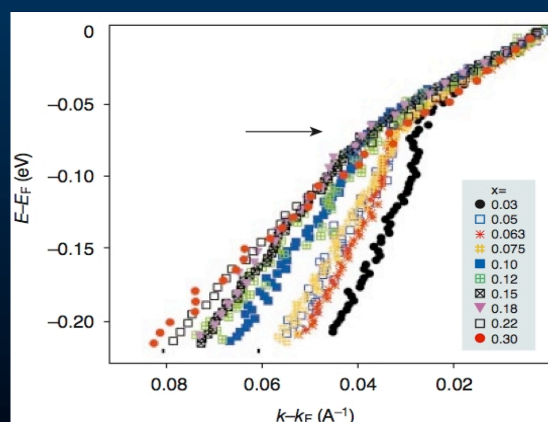
“Ubiquitous”

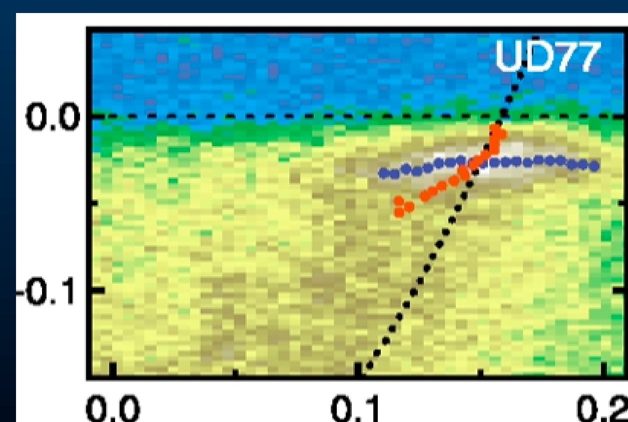








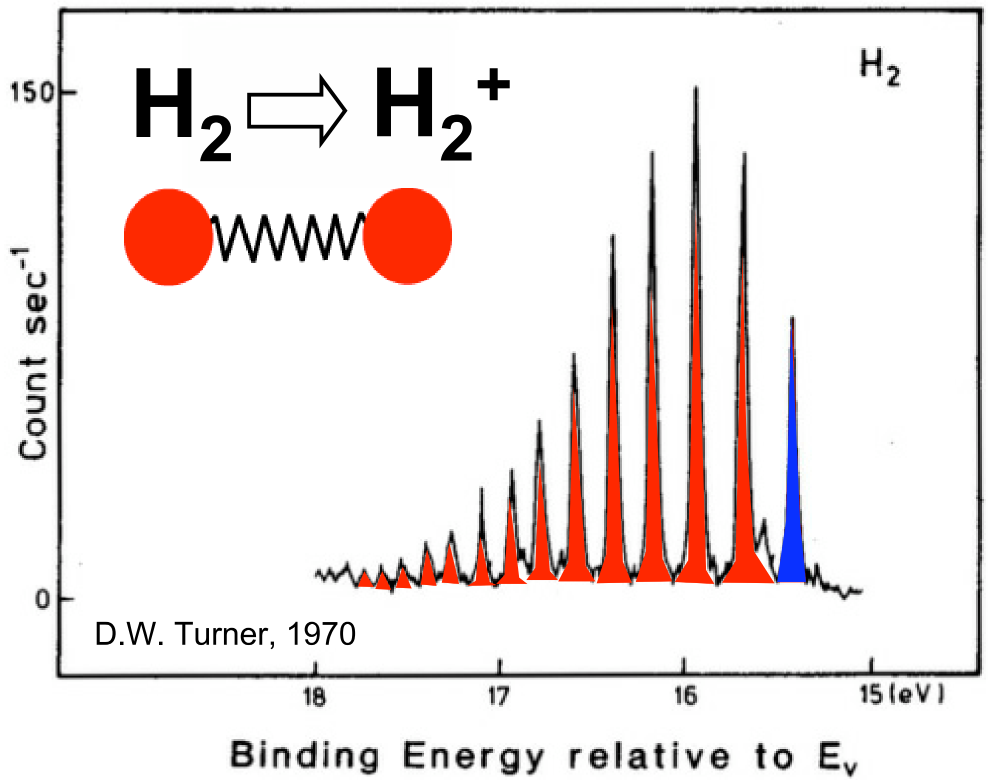




Campuzano, Dessau, Fink, Johnson, Lanzara, Norman, Z.-X. Shen, Takahashi

Franck-Condon Effect

$$\mathcal{H} = \epsilon_0\, c^\dagger c + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + \sqrt{g\omega_0^2}\, \sum_{\mathbf{q}} c^\dagger c (a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}})$$



Equivalent to Franck-Condon broadening

Comparison with Fermi Liquid

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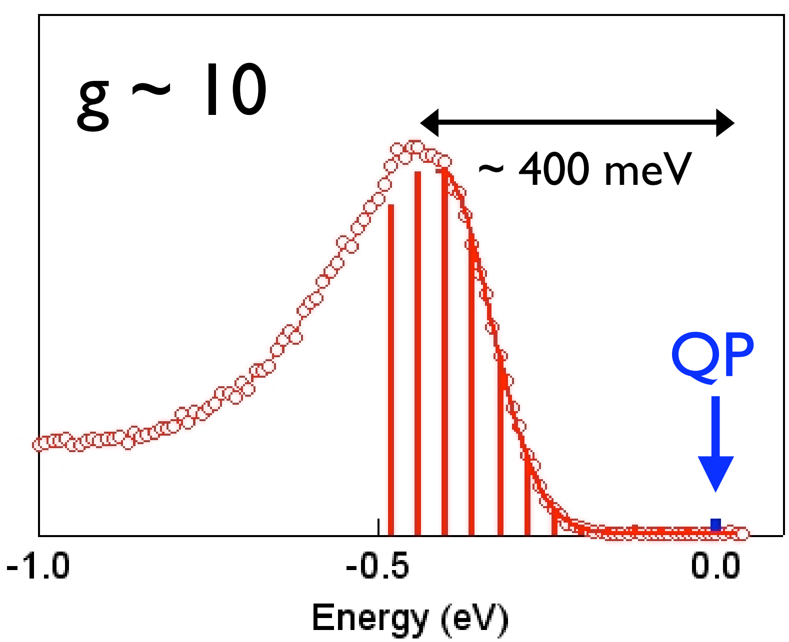

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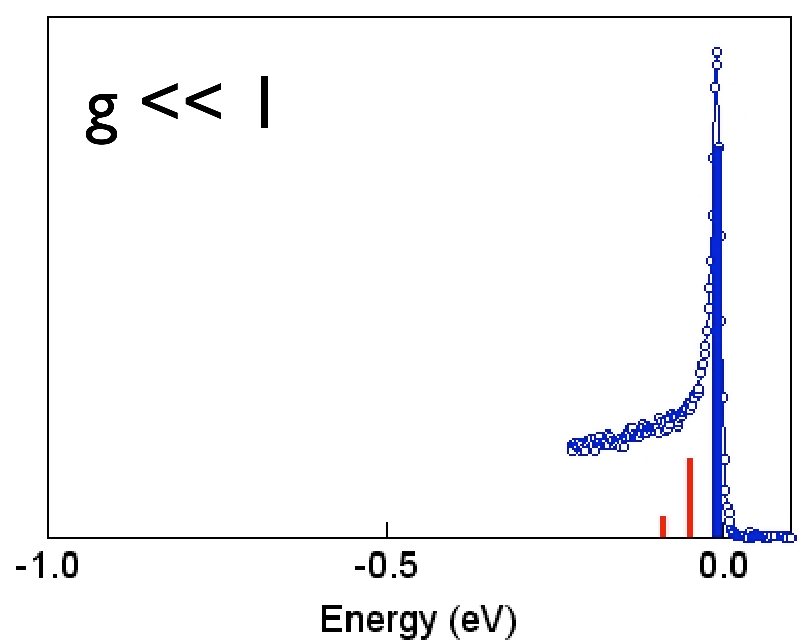
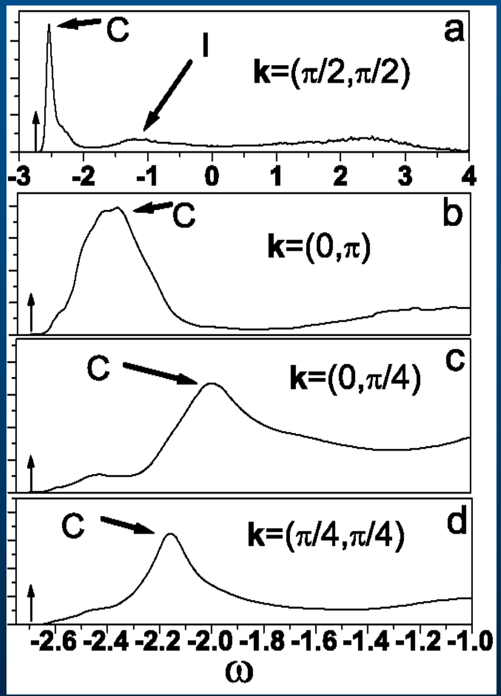


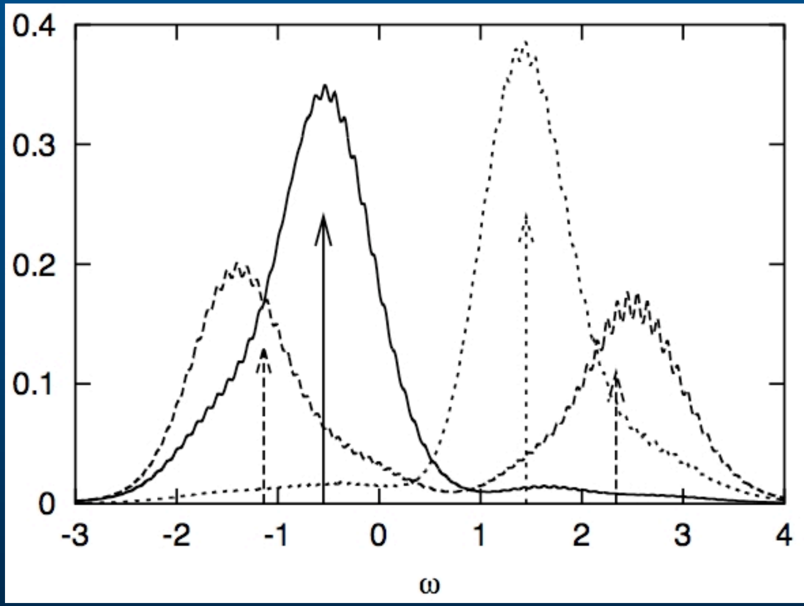
Theoretical Treatments of Polaron Physics

A. Mishchenko & N. Nagaosa



Phys. Rev. Lett. 93, 046402 (2004)

O. Rosch & O. Gunnarsson



Euro. Phys. J B (2005)

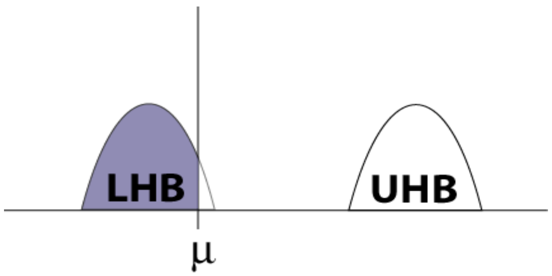
Centroid (first moment) of spectral weight tracks "frozen lattice" dispersion!

Doping Evolution of the Cuprates

Emergence of the Sharp Nodal Quasiparticles

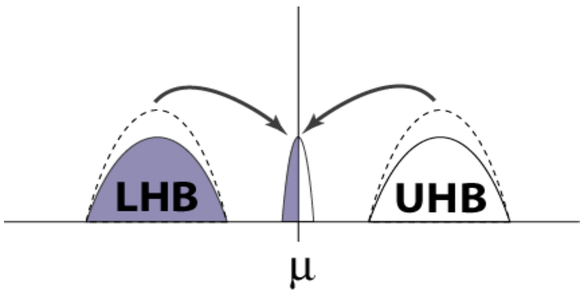
Resolving the Long-Standing Controversy over the Doping Evolution of the Chemical Potential

Shift into LHB / UHB



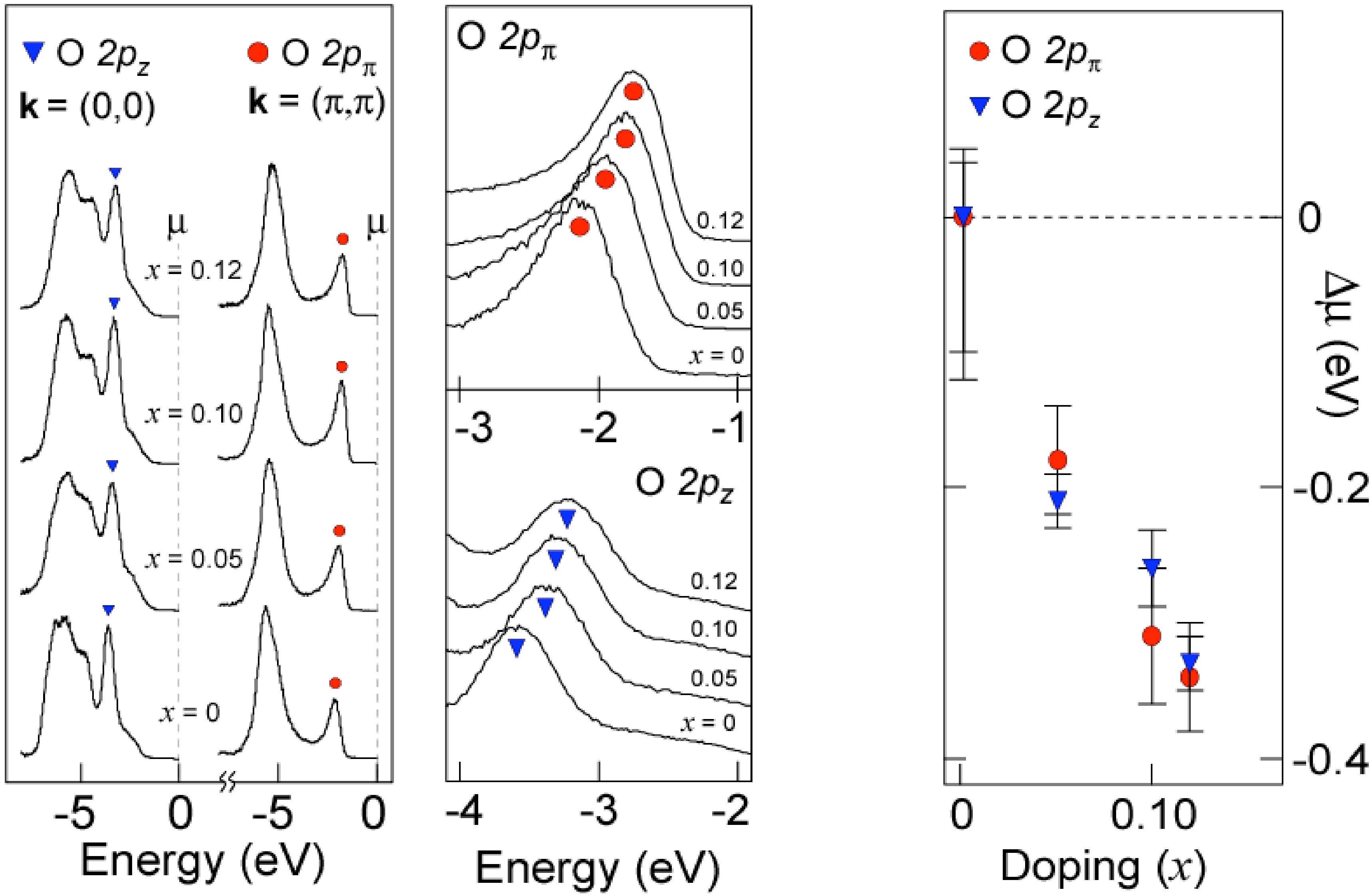
Z.-X. Shen *et al.*, PRB **44**, 12098
P.G. Steeneken *et al.*, PRL **90**, 247005
N.P. Armitage *et al.*, PRL **88**, 257001
Y. Kohsaka *et al.*, JPSJ **72**, 1018

Midgap States

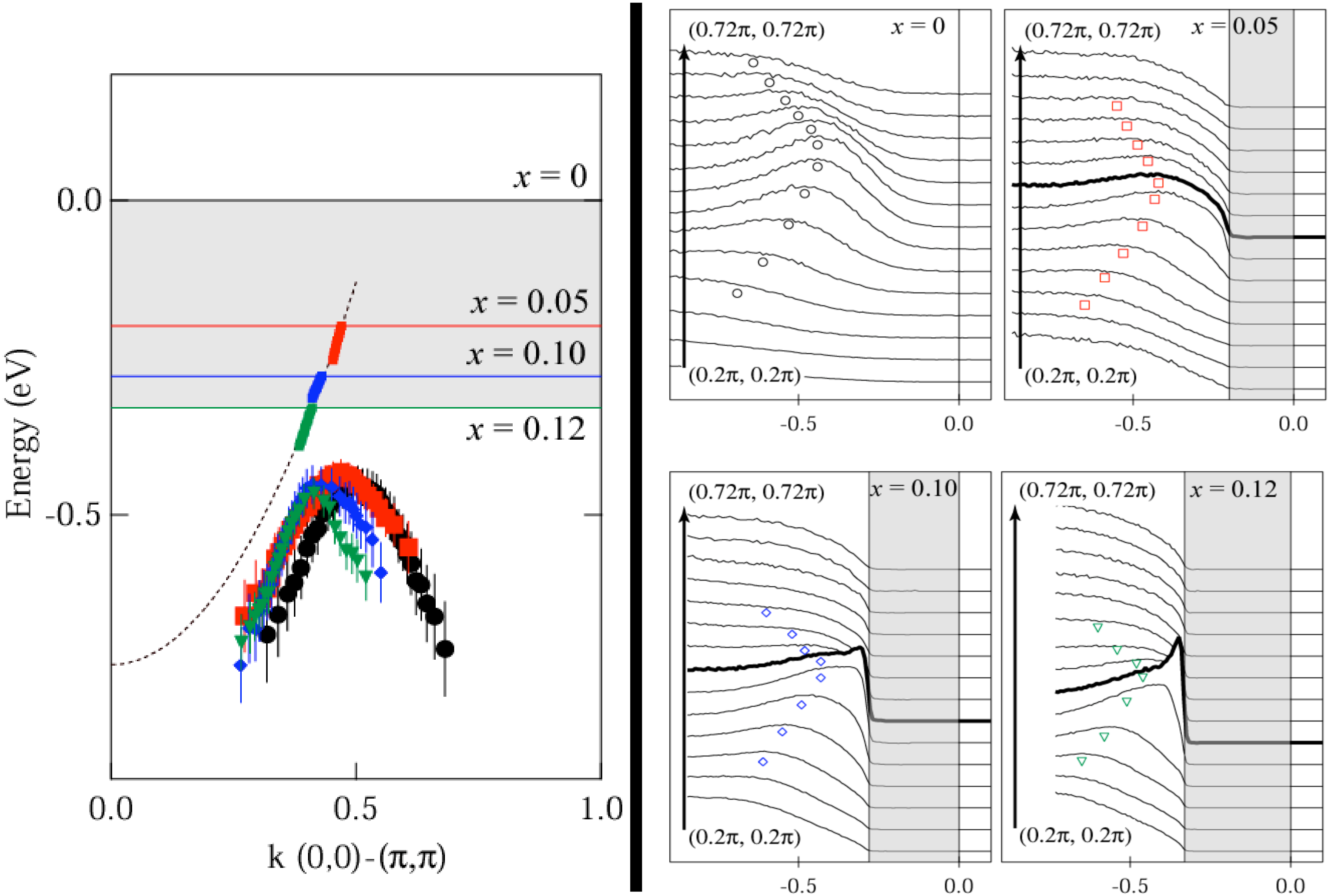


J.W. Allen *et al.*, PRL **64**, 595
R.O. Anderson *et al.*, PRL **70**, 3163
A. Ino *et al.*, PRL **79**, 2101
N. Harima *et al.*, PRB **64**, 220507

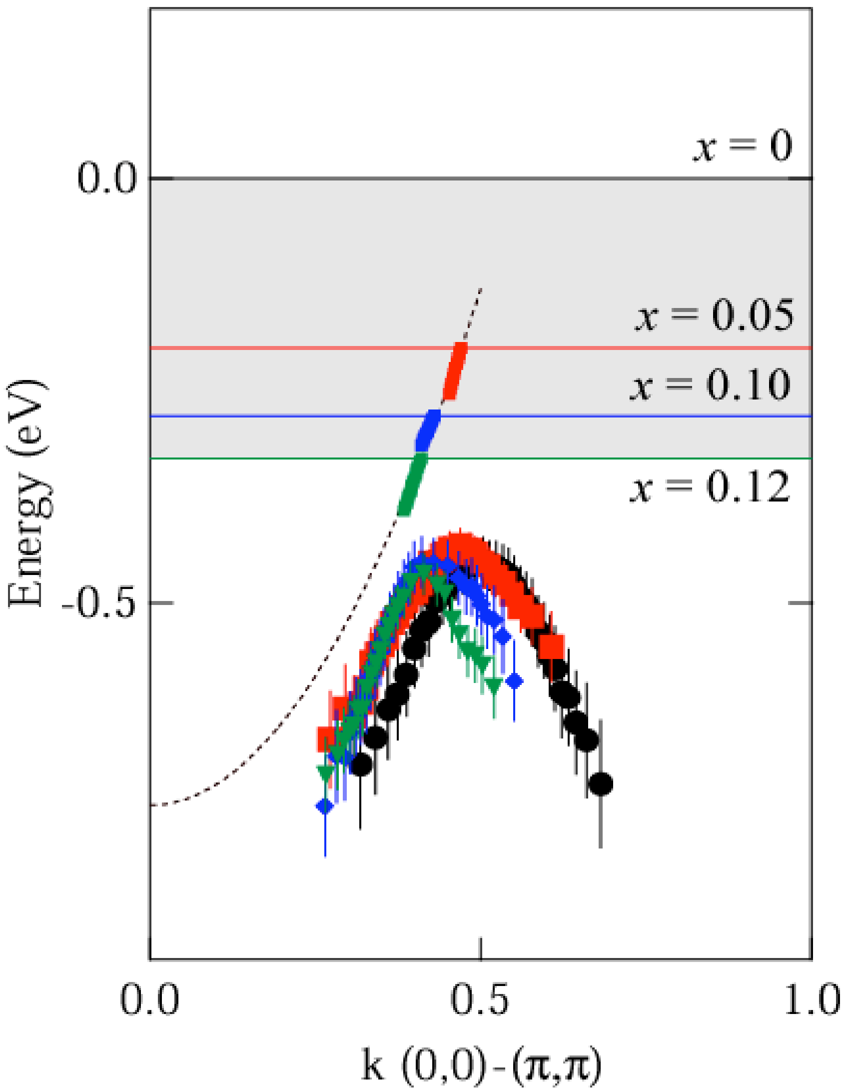
Chemical Potential Shift : O2p_π & O2p_z

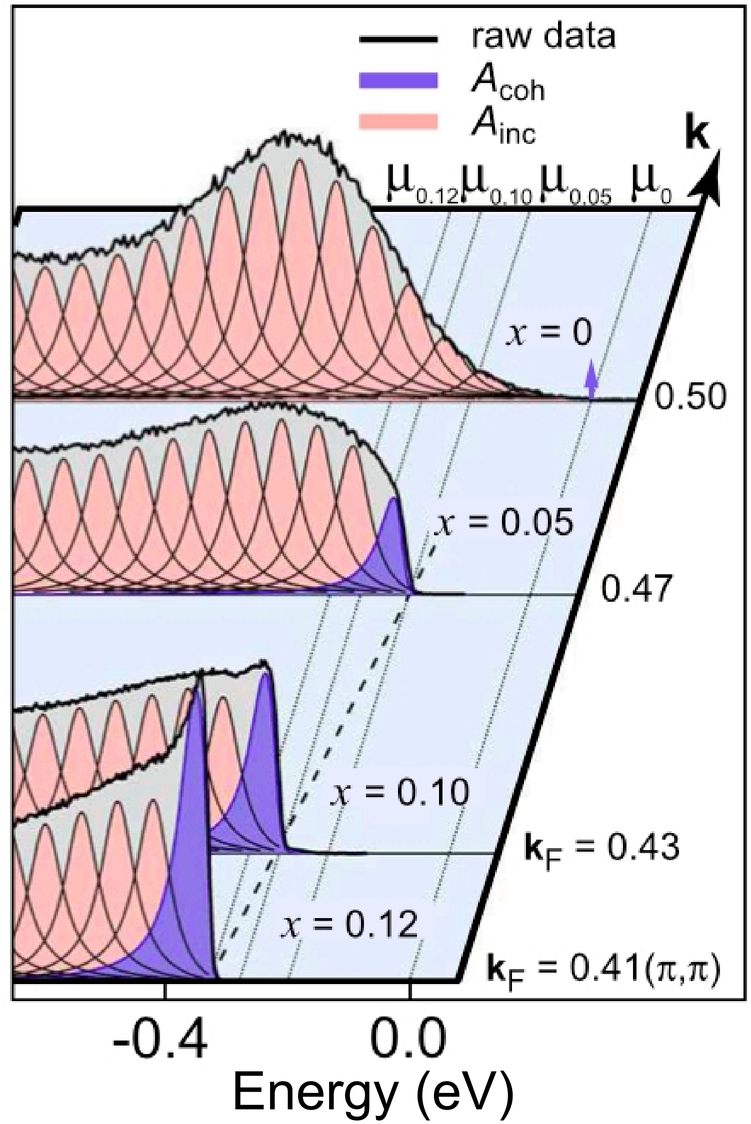


Evolution of Low Energy States

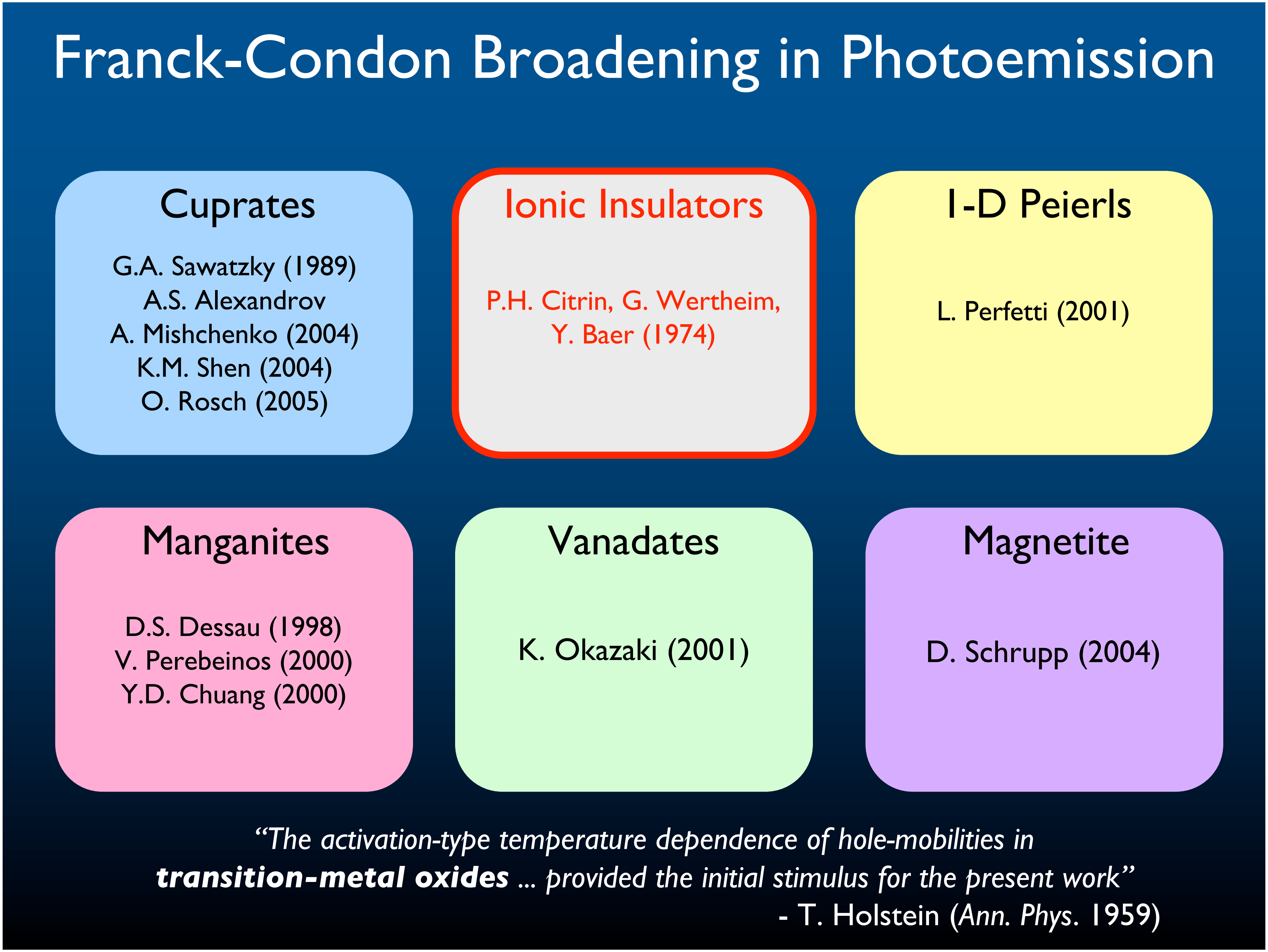


Evolution of Low Energy States



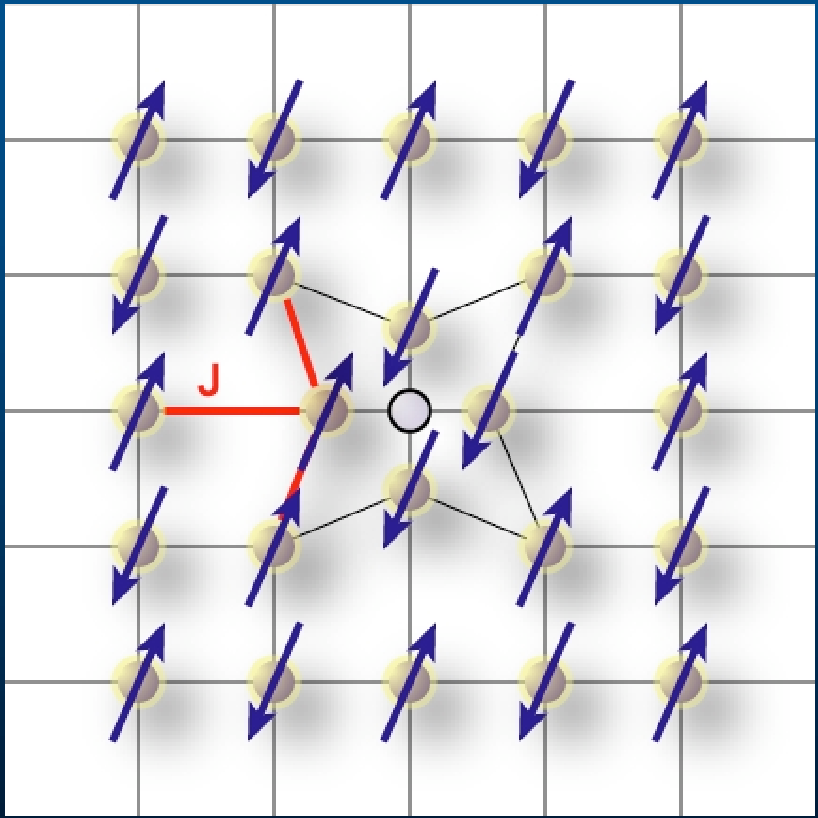


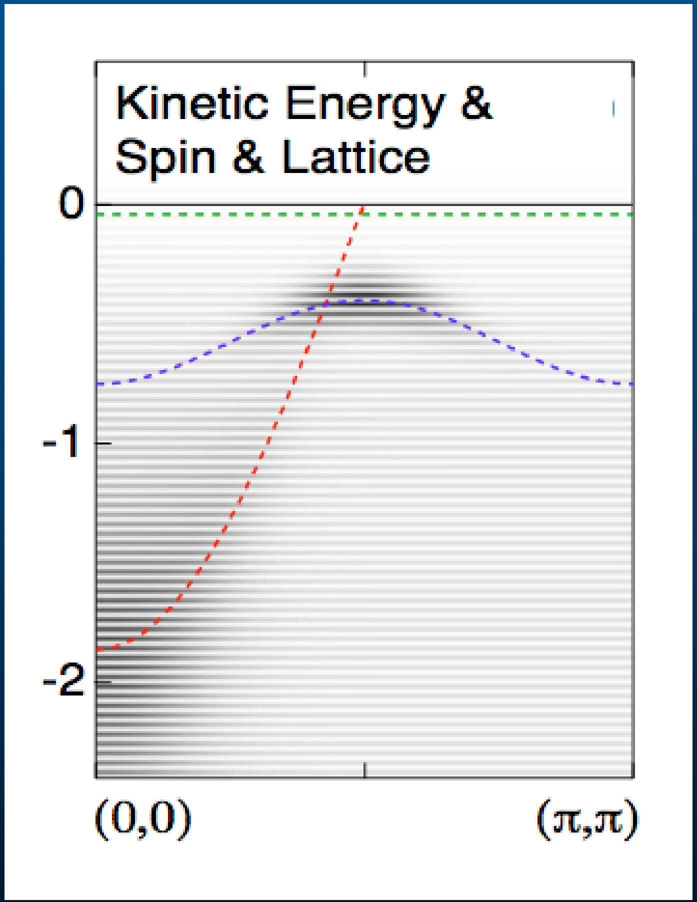
K.M. Shen, *et al.*, PRL 93, 267002 (2004)


Franck-Condon Broadening in Photoemission
Cuprates
G.A. Sawatzky (1989)
A.S. Alexandrov
A. Mishchenko (2004)
K.M. Shen (2004)
O. Rosch (2005)
Ionic Insulators
P.H. Citrin, G. Wertheim, Y. Baer (1974)
1-D Peierls
L. Perfetti (2001)
Manganites
D.S. Dessau (1998)
V. Perebeinos (2000)
Y.D. Chuang (2000)
Vanadates
K. Okazaki (2001)
Magnetite
D. Schrupp (2004)
"The activation-type temperature dependence of hole-mobilities in transition-metal oxides ... provided the initial stimulus for the present work"
- T. Holstein (Ann. Phys. 1959)

Strong Interactions in the Cuprates

KE & Magnetism & Lattice

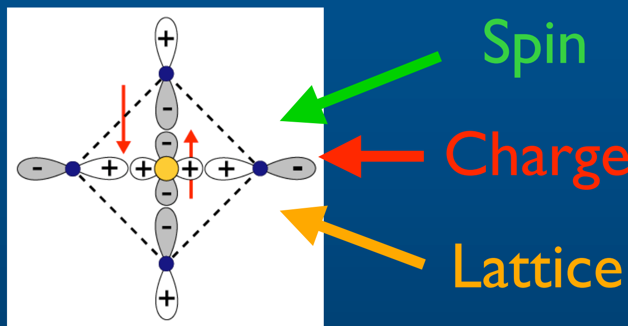




A.S. Mishchenko & N. Nagaosa (PRL '04);
O. Rosch & O. Gunnarsson (PRL '04, EPJ B '05)

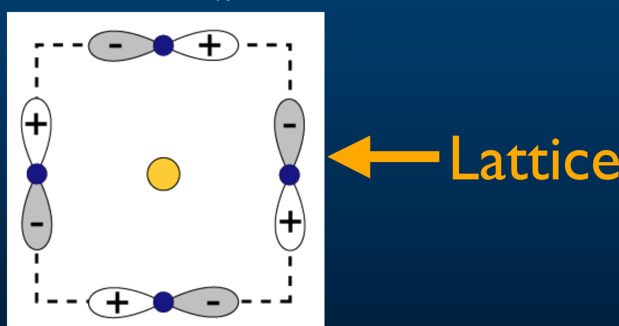
Determining the Origin of Broadening

Lower Hubbard Band



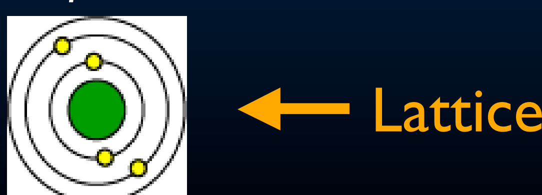
LHB states tied to spin, charge, and lattice degrees of freedoms

O $2p_{\pi}$



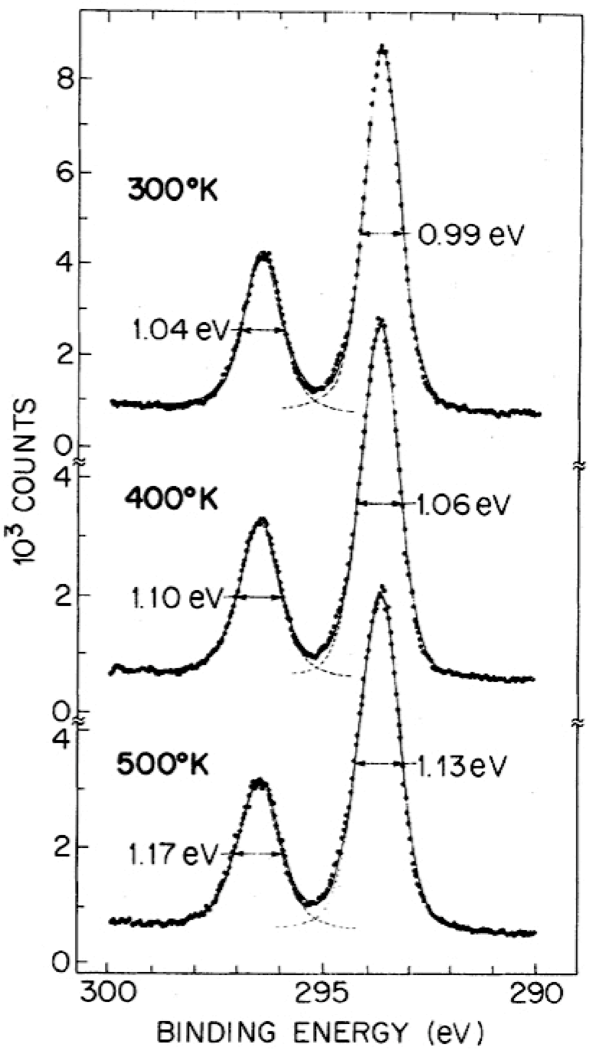
O $2p_{\pi}$ and Ca *3p* states have *no overlap* with LHB or Cu *3d* orbitals. Therefore, represents primarily lattice contribution

Ca *3p* Core



Use these states as a simple benchmark!

Franck-Condon Broadening : Core Levels



P.H. Citrin *et al.*, PRL (1974)
also G.K. Wertheim & Y. Baer

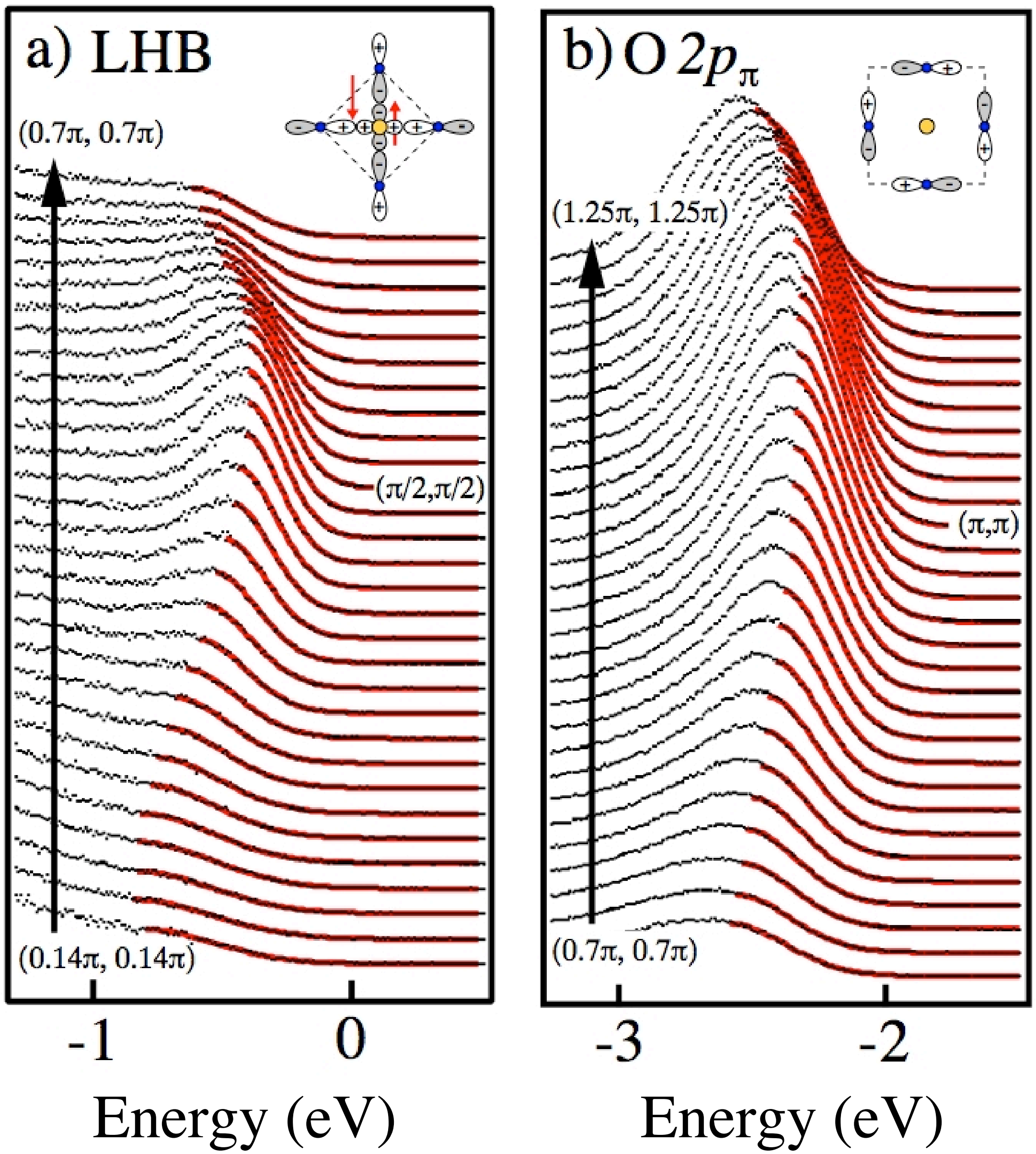
Core Hole lifetimes in Alkali Halides (KCl, KI, KF)

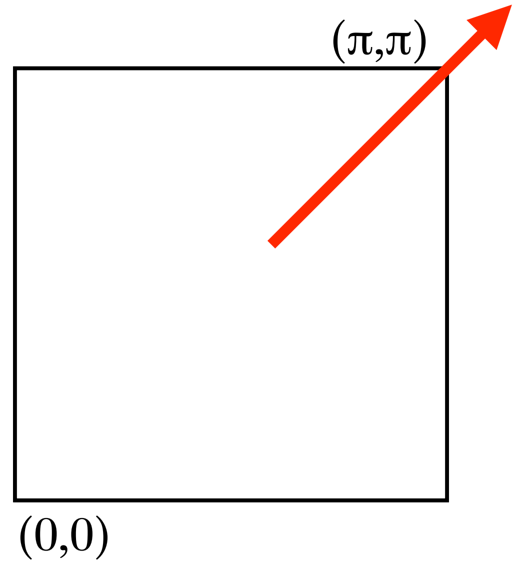
• Lineshape and temperature dependence in ionic insulators very different from simple metals

• Gaussian lineshapes suggested lattice (Franck-Condon) broadening dominant

• Significant temperature broadening (unexpected from electron-hole decay)

Comparison of Lineshape





- Both LHB & O2p_π states exhibit Gaussian lineshapes
- Franck-Condon Broadening exists for uncorrelated non-LHB state (O2p_π)

K.M. Shen *et al.*, submitted
J.J.M. Pothuizen *et al.*, PRL (1997)

Acknowledgements

Stanford University (ARPES) : Filip Ronning, Donghui Lu, Weisheng Lee, Nicholas Ingle, Felix Baumberger, Worawat Meevasana, and Z.-X. Shen

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Kyoto University (Samples) : Masaki Azuma and Mikio Takano

University of Oregon (Samples) : Lance Miller

Helpful Discussions : N.P. Armitage, A. Damascelli, J.C. Davis, A. Fujimori, T. Hanaguri, D.H. Lee, A. Mishchenko, N. Nagaosa, G.A. Sawatzky

Conclusions

- Spectral features of insulating cuprates (and many TMOs!) can be understood in a polaronic / Franck-Condon model
- Quasiparticles grow from near zero intensity when doped away from insulator, and this QP band controls μ
- FCB present in other uncorrelated electronic states, suggesting a strong lattice contribution

K.M. Shen *et al.*, Phys. Rev. Lett. 93, 267002 (2004)
K.M. Shen *et al.*, Science 307, 901 (2005)
K.M. Shen *et al.*, submitted (2005)