# Condensed Matter Physics II
# SS 2015

Wednesday 9:30-12:30

Seminar Room Physics 2

Prof. Paul H.M. van Loosdrecht

pvl@ph2.uni-koeln.de

www.loosdrecht.net

VOLUME 3, NUMBER 1 PHYSICAL REVIEW LETTERS JULY 1, 1959

# OXIDES WHICH SHOW A METAL-TO-INSULATOR TRANSITION AT THE NEEL TEMPERATURE

F. J. Morin
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received June 5, 1959)

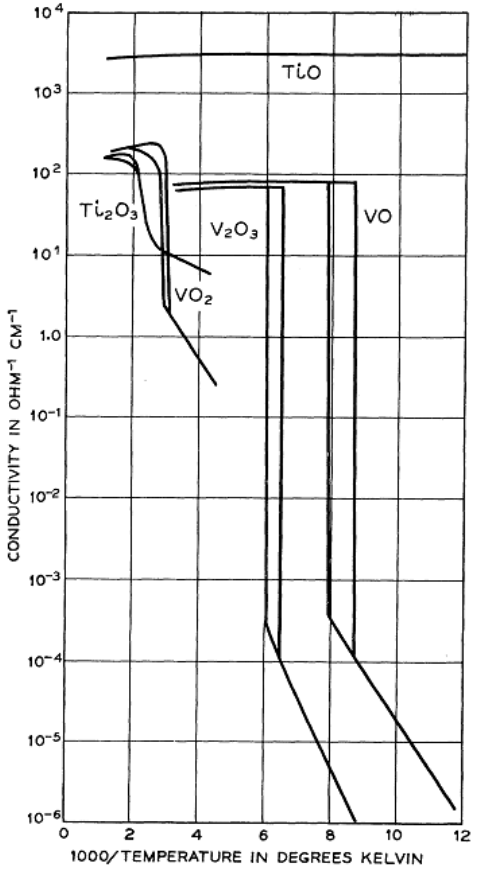


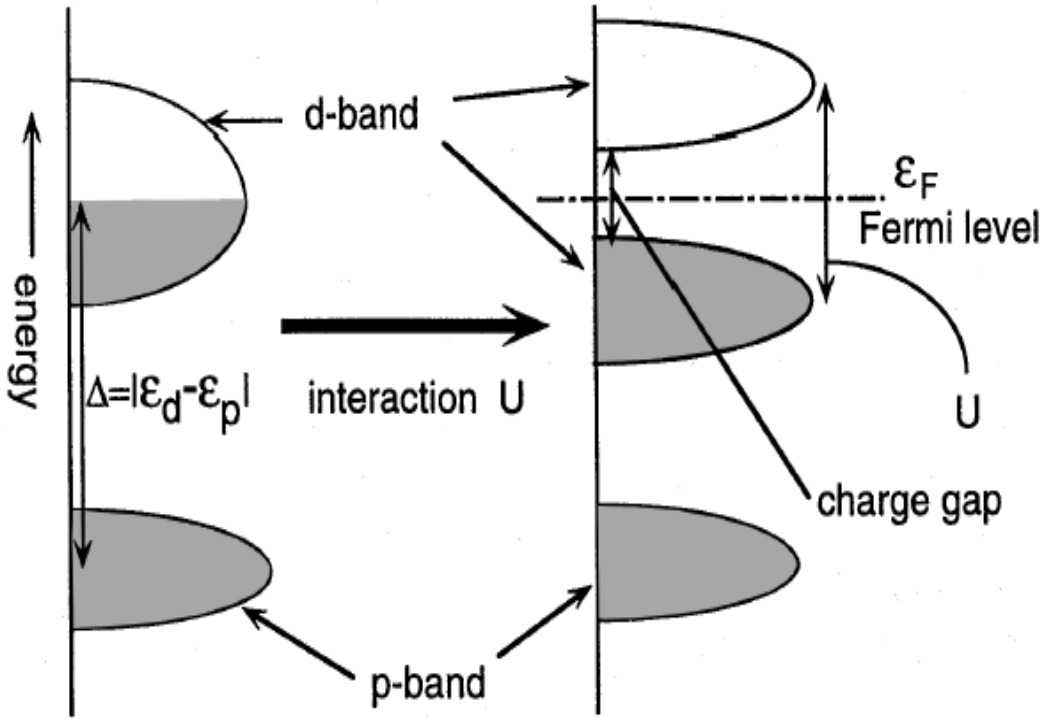

FIG. 1. Conductivity as a function of reciprocal temperature for the lower oxides of titanium and vanadium. Measurements were made along the [100] direction in VO, and along the $c$ axis in $V_2O_3$ and $VO_2$.

$VO_2$

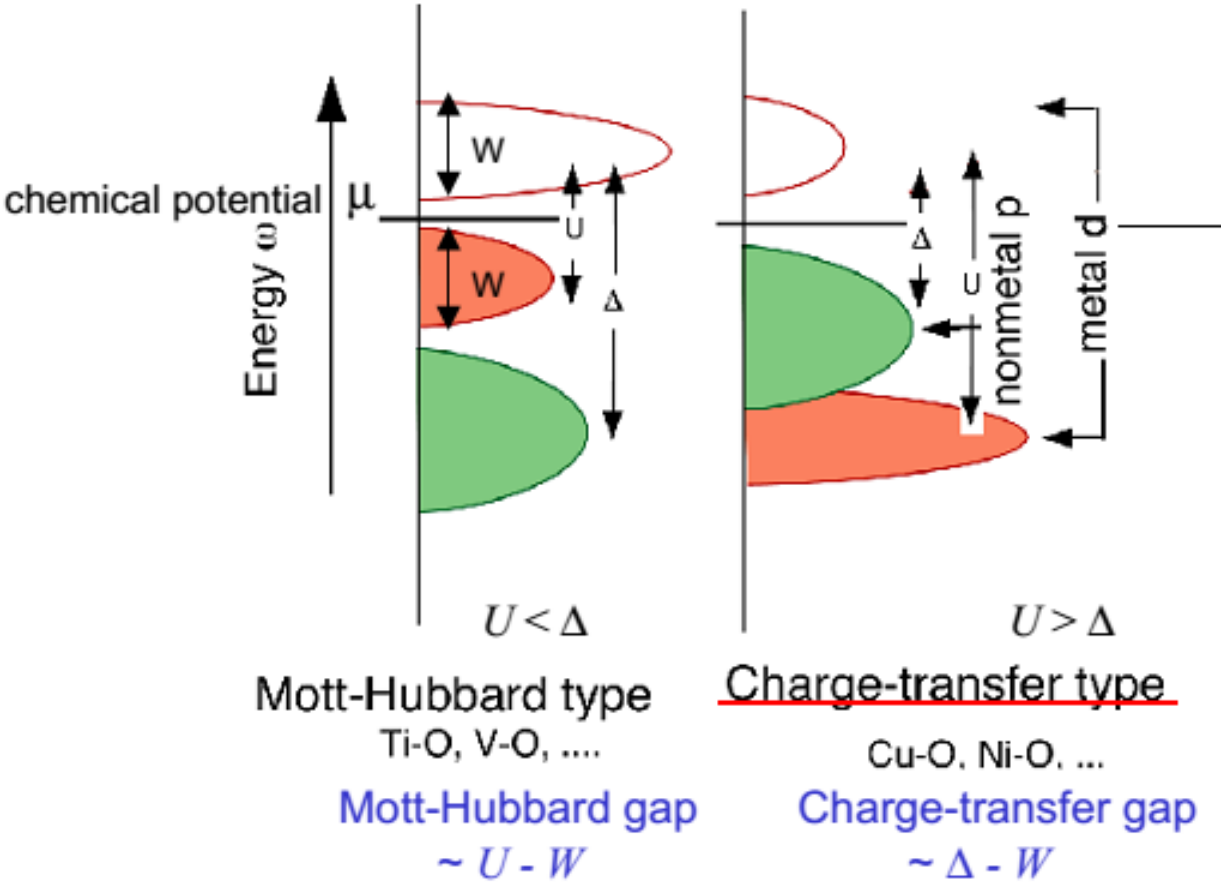
Metal-Insulator transition at 340 K, also structural change:low T monoclinic, high T tetragonal (rutile) !!

Band insulator?
Mott Hubbard insulator?

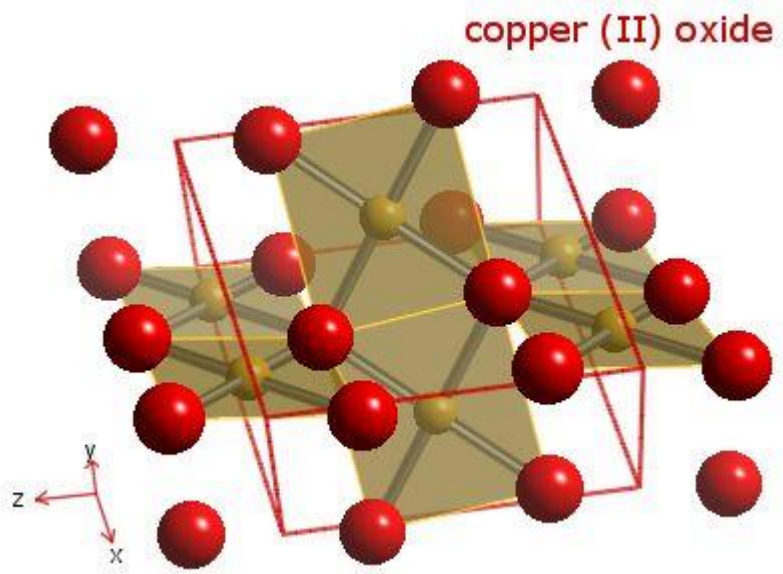
Valence electrons V: $3d^3 4s^2$
So $V^{4+}$ : $3d^1$

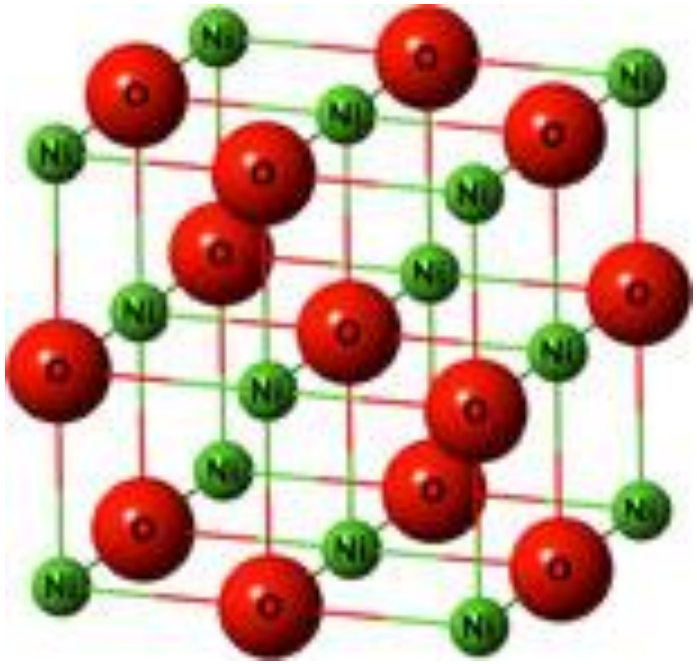

d-band
energy
Δ=|ε_d-ε_p|
interaction U
ε_F
Fermi level
U
charge gap
p-band

# Mott vs Charge transfer



# CuO & NiO



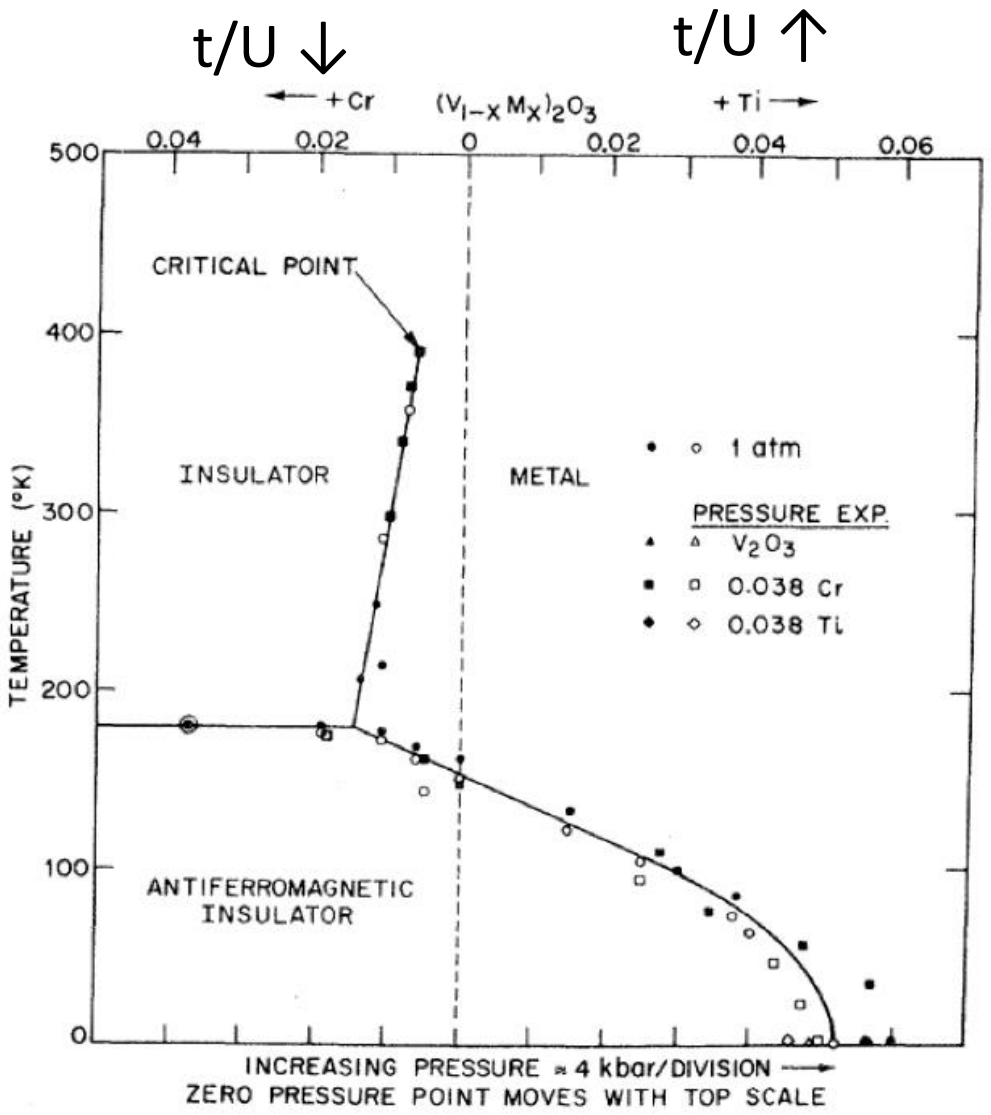




CuO

NiO

$Cu^{2+}$: [Ar] $3d^9$

$Ni^{2+}$: [Ar] $3d^8$




from McWhan *et al.*, Phys. Rev. B (1973)

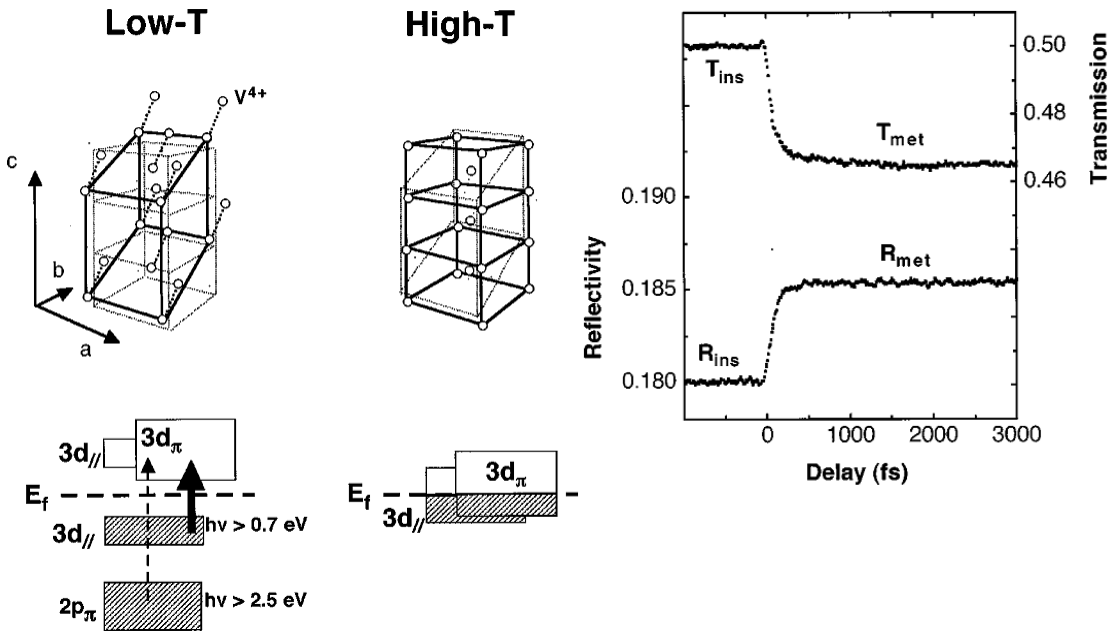
U↑ →

U↓

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sc$^{21}$ $3d\ 4s^2$ | Ti$^{22}$ $3d^2\ 4s^2$ | V$^{23}$ $3d^3\ 4s^2$ | Cr$^{24}$ $3d^5\ 4s$ | Mn$^{25}$ $3d^5\ 4s^2$ | Fe$^{26}$ $3d^6\ 4s^2$ | Co$^{27}$ $3d^7\ 4s^2$ | Ni$^{28}$ $3d^8\ 4s^2$ | Cu$^{29}$ $3d^{10}\ 4s$ | Zn$^{30}$ $3d^{10}\ 4s^2$ |
| Y$^{39}$ $4d\ 5s^2$ | Zr$^{40}$ $4d^2\ 5s^2$ | Nb$^{41}$ $4d^4\ 5s$ | Mo$^{42}$ $4d^5\ 5s$ | Tc$^{43}$ $4d^6\ 5s$ | Ru$^{44}$ $4d^7\ 5s$ | Rh$^{45}$ $4d^8\ 5s$ | Pd$^{46}$ $4d^{10}$ – | Ag$^{47}$ $4d^{10}\ 5s$ | Cd$^{48}$ $4d^{10}\ 5s^2$ |
| La$^{57}$ $5d\ 6s^2$ | Hf$^{72}$ $4f^{14}\ 5d^2\ 6s^2$ | Ta$^{73}$ $5d^3\ 6s^2$ | W$^{74}$ $5d^4\ 6s^2$ | Re$^{75}$ $5d^5\ 6s^2$ | Os$^{76}$ $5d^6\ 6s^2$ | Ir$^{77}$ $5d^9$ – | Pt$^{78}$ $5d^9\ 6s$ | Au$^{79}$ $5d^{10}\ 6s$ | Hg$^{80}$ $5d^{10}\ 6s^2$ |
| Ac$^{89}$ $6d\ 7s^2$ | Ce$^{58}$ $4f^2\ 6s^2$ | Pr$^{59}$ $4f^3\ 6s^2$ | Nd$^{60}$ $4f^4\ 6s^2$ | Pm$^{61}$ $4f^5\ 6s^2$ | Sm$^{62}$ $4f^6\ 6s^2$ | Eu$^{63}$ $4f^7\ 6s^2$ | Gd$^{64}$ $4f^7\ 5d\ 6s^2$ | Tb$^{65}$ $4f^8\ 5d\ 6s^2$ | |
| | Th$^{90}$ – $6d^2\ 7s^2$ | Pa$^{91}$ $5f^2\ 6d\ 7s^2$ | U$^{92}$ $5f^3\ 6d\ 7s^2$ | Np$^{93}$ $5f^5\ 7s^2$ | Pu$^{94}$ $5f^6\ 7s^2$ | Am$^{95}$ $5f^7\ 7s^2$ | Cm$^{96}$ $5f^7\ 6d\ 7s^2$ | Bk$^{97}$ | |

# Evidence for a structurally-driven insulator-to-metal transition in $VO_2$: A view from the ultrafast timescale

A. Cavalleri,[1,*] Th. Dekorsy,[2] H. H. W. Chong,[1] J. C. Kieffer,[3] and R. W. Schoenlein[1]
[1]*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA*
[2]*Forschungszentrum Rossendorf, Dresden, Germany*
[3]*INRS énergie et matériaux, Université du Québec, Varennes, Québec, Canada*
(Received 4 September 2003; revised manuscript received 1 July 2004; published 13 October 2004)



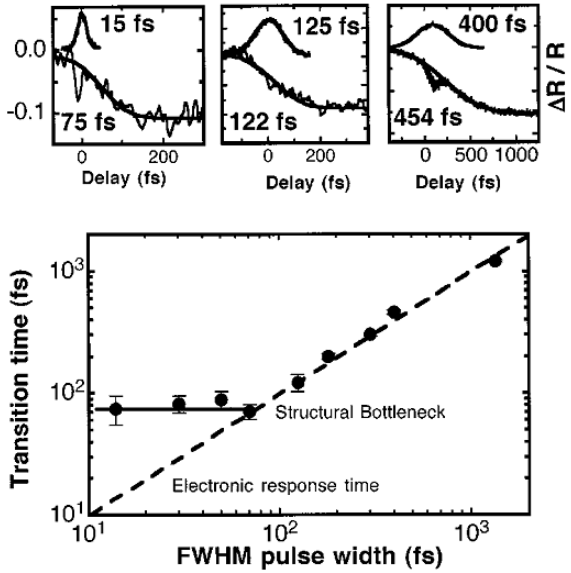



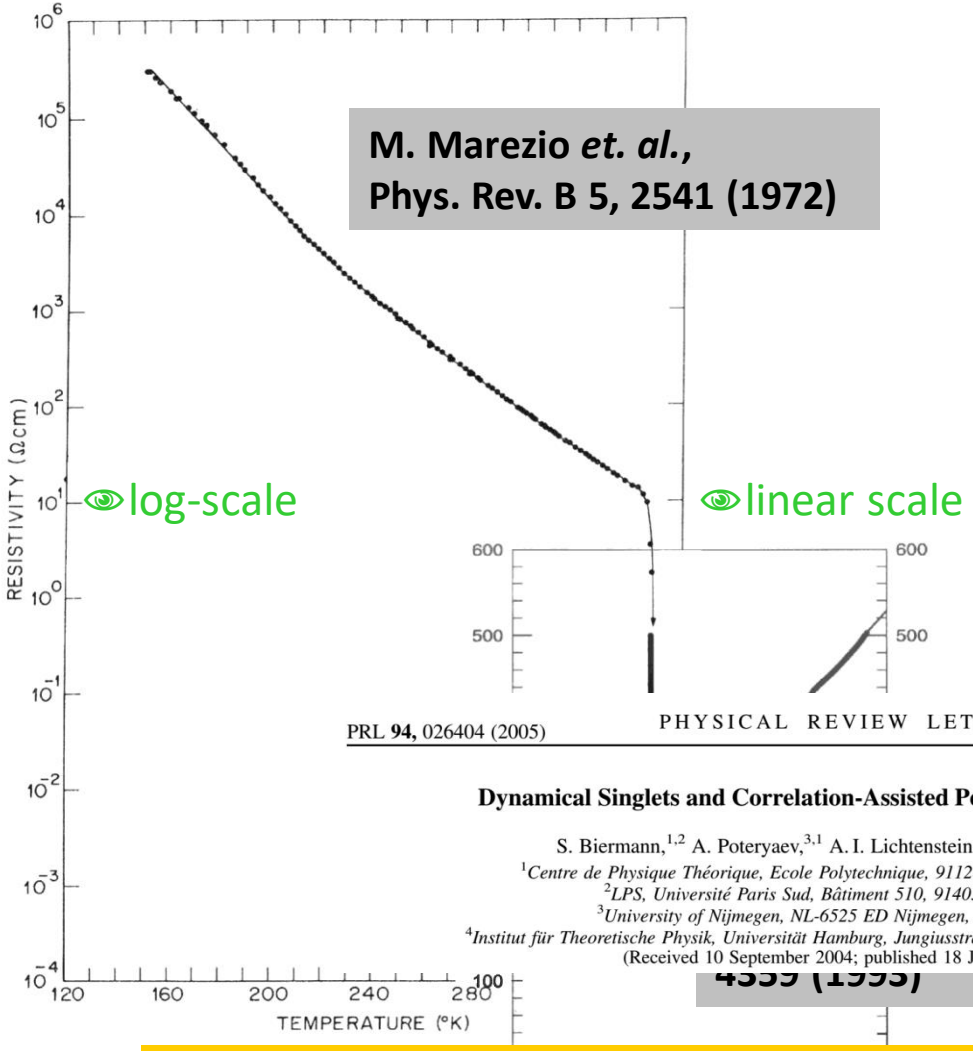

FIG. 3. Pump-probe reflectivity experiments of the photoinduced phase transition. The experiments are performed in the nonetched structure with variable pulse durations between 1.5 ps and 15 fs, as measured at the sample position. White light was amplified in 1-mm, 32°-cut BBO, pumped with 400-nm pulses crossing the seed light at 3.5°. Pulse compression in a pair of prisms was used to minimize the duration of the pump-probe autocorrelation at the sample position. The experiments were conducted using pulses of 100-nm bandwidth full width at half maximum centered around 650 nm.

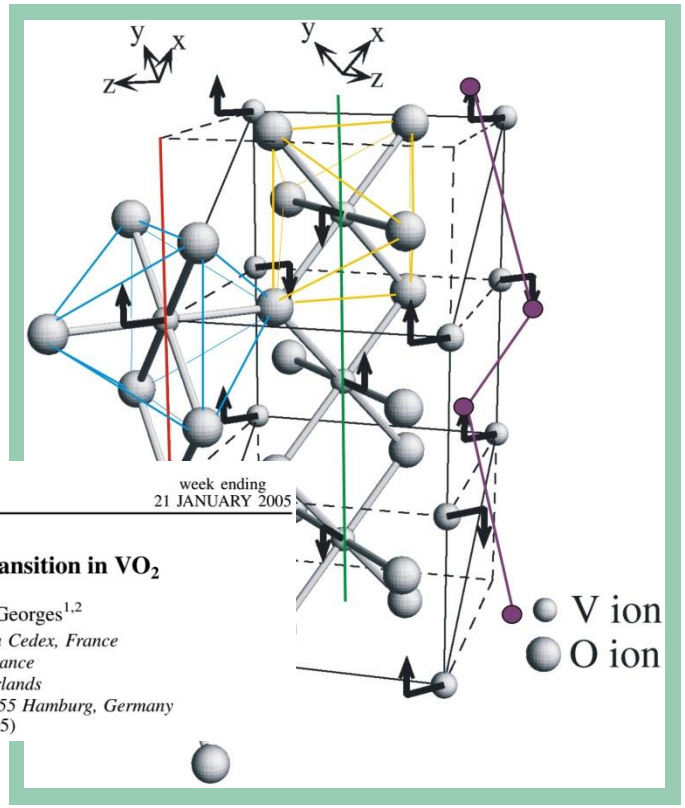
# Metal insulator transition in $VO_2$ at 340 K

***T* > 340K**: metal, rutile

***T* < 340K**: insulator, monoclinic, dimerized zig-zag chain

M. Marezio *et. al.*,
Phys. Rev. B 5, 2541 (1972)



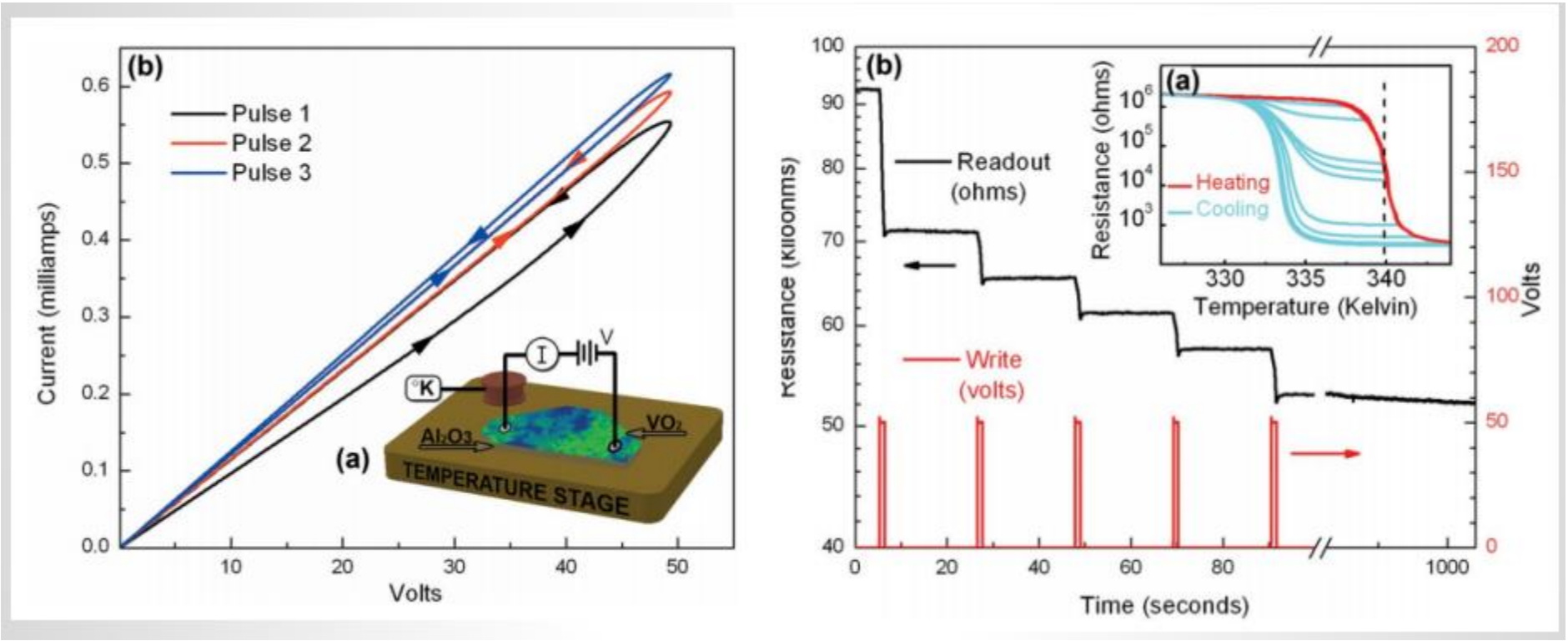

PRL 94, 026404 (2005) PHYSICAL REVIEW LETTERS week ending 21 JANUARY 2005

**Dynamical Singlets and Correlation-Assisted Peierls Transition in $VO_2$**

S. Biermann,[1,2] A. Poteryaev,[3,1] A. I. Lichtenstein,[4] and A. Georges[1,2]
[1]*Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France*
[2]*LPS, Université Paris Sud, Bâtiment 510, 91405 Orsay, France*
[3]*University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands*
[4]*Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*
(Received 10 September 2004; published 18 January 2005)

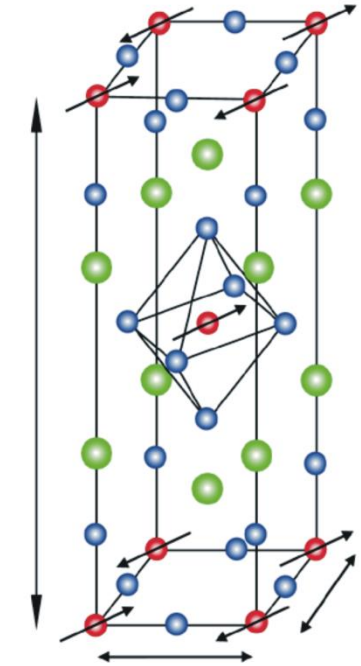
Dimerization → Peierls transition = band structure effect
Combination of Peierls and Hubbard physics

# $VO_2$ Memristors

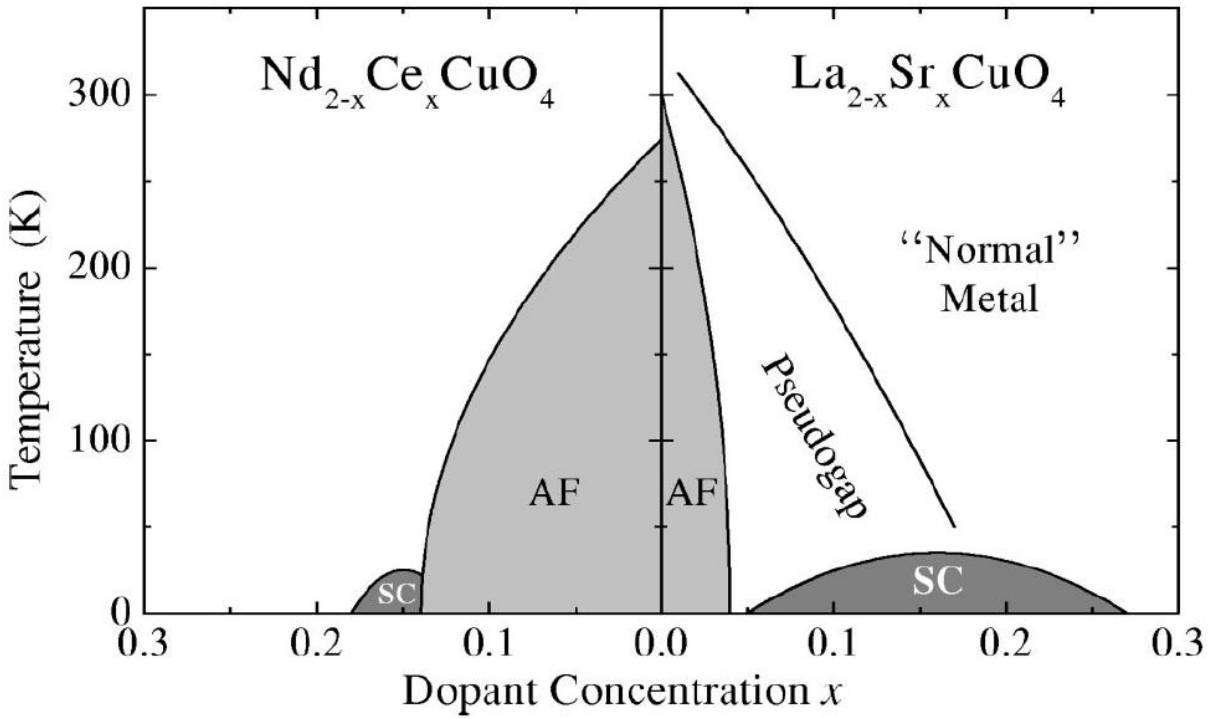



Driscoll, T., Applied Physics Letters 95 (2009)

# High temperature superconductivity

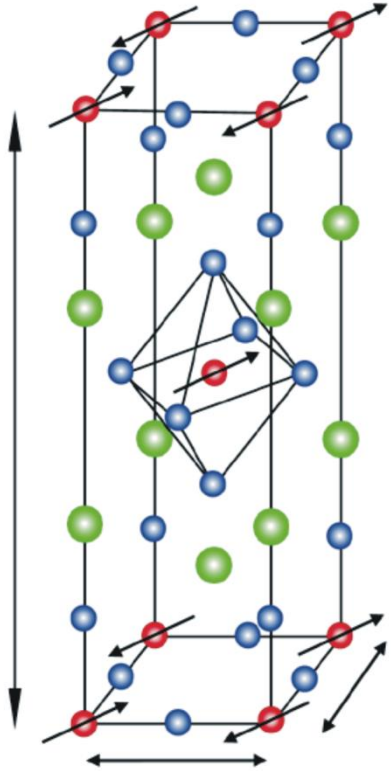


$Cu^{2+}$
$O^{2-}$
$La^{3+}$




Adapted from Patrick Lee and T. Senthil

# CuO plane: strongly-correlated electron system



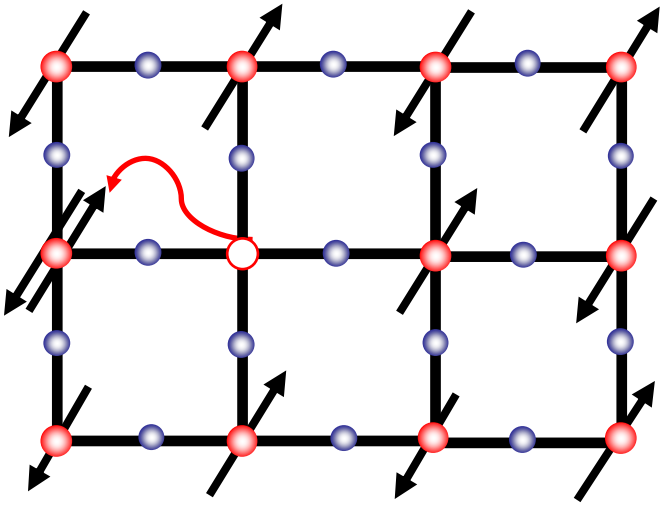
$Cu^{2+}$

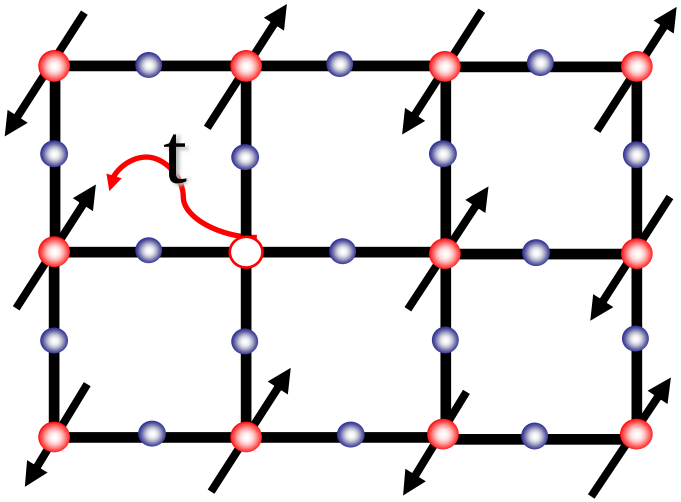
$O^{2-}$

$La^{3+}$

One hole per site: should be a metal according to band theory.

Mott insulator.



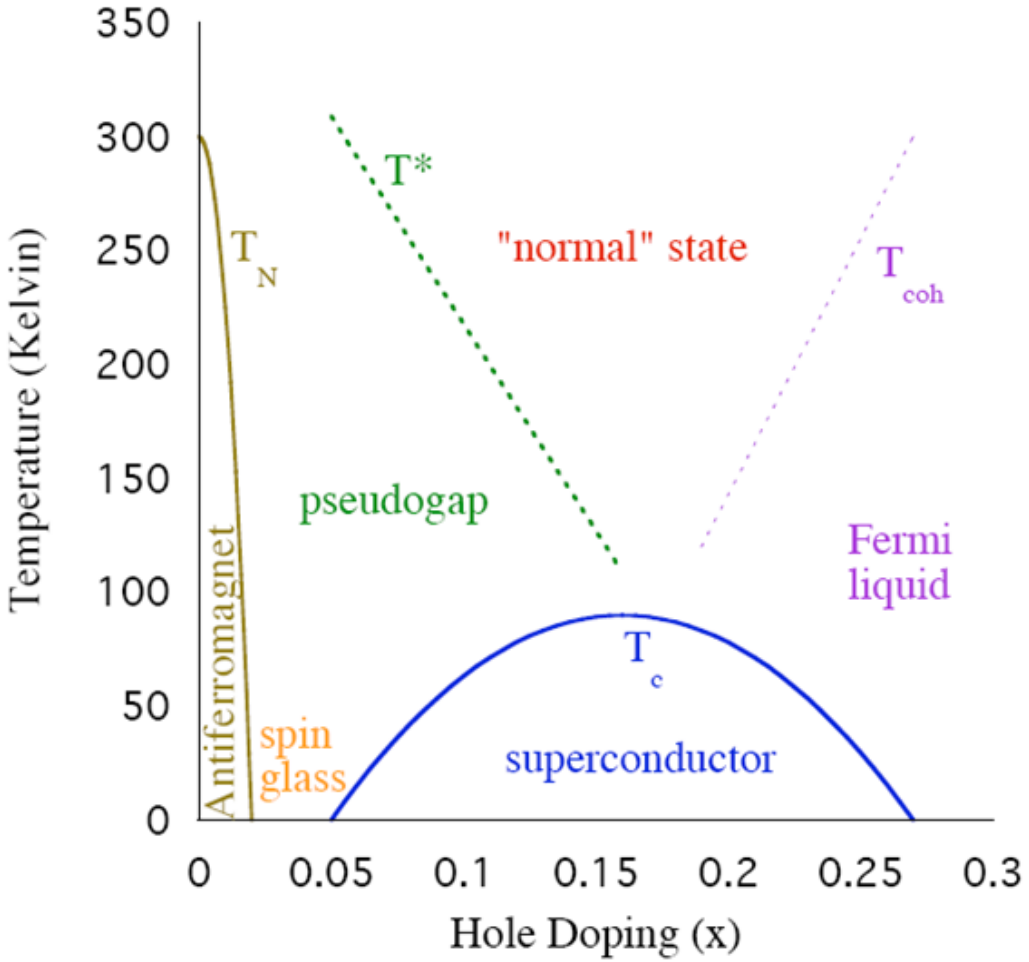



*Undoped $CuO_2$ plane: Mott Insulator due to $e^-$ - $e^-$ interaction Virtual hopping induces AF exchange $J=4t^2/U$*

*$CuO_2$ plane with doped holes:*

$La^{3+} \rightarrow Sr^{2+}$: $La_{2-x}Sr_xCuO_4$

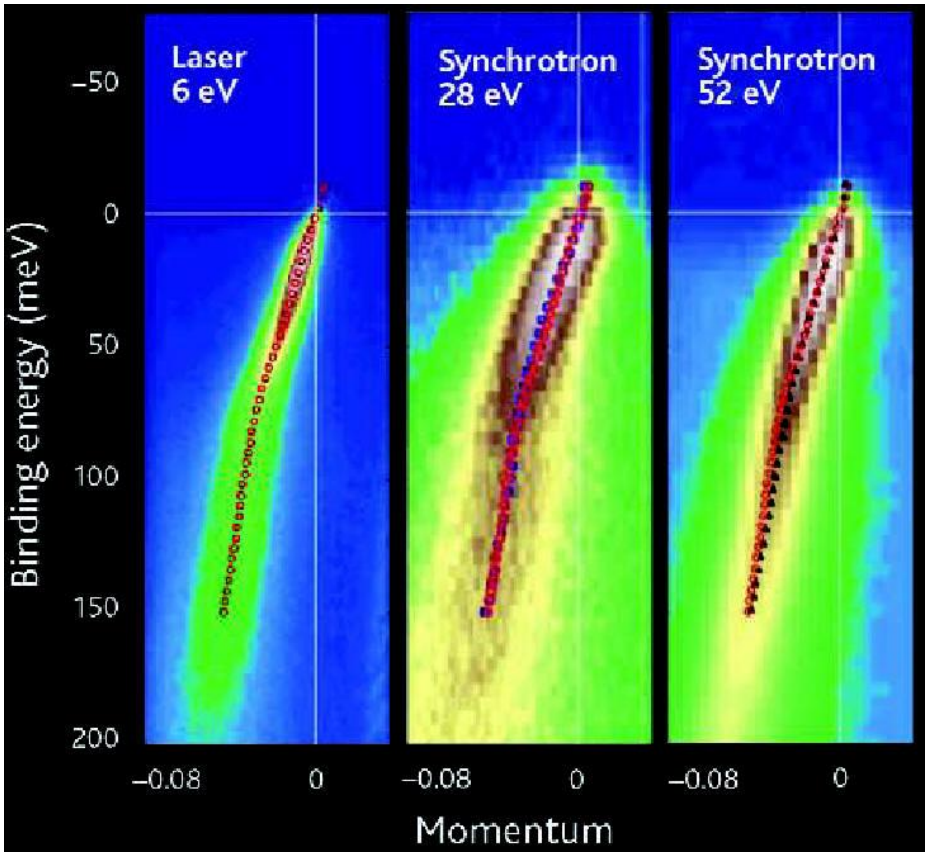
Adapted from Patrick Lee and T. Senthil



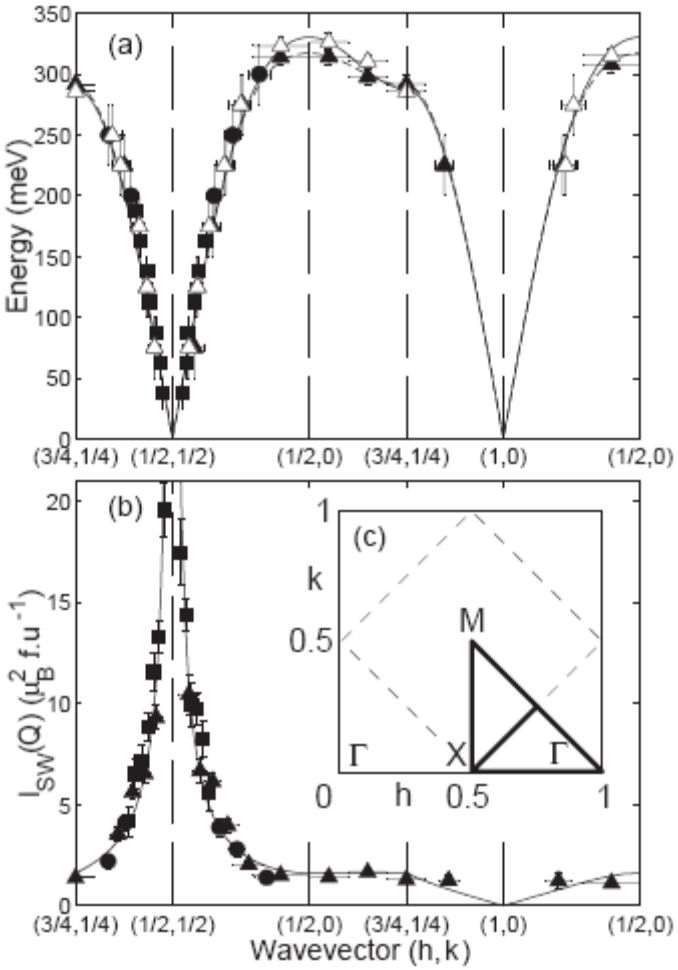

Adapted from Patrick Lee and T. Senthil

# Laser Based Angle-Resolved Photoemission, the Sudden Approximation, and Quasiparticle-Like Spectral Peaks in $Bi_2Sr_2CaCu_2O_{8+\delta}$

J. D. Koralek,[1,2,*] J. F. Douglas,[1] N. C. Plumb,[1] Z. Sun,[1,3] A. V. Fedorov,[3] M. M. Murnane,[1,2] H. C. Kapteyn,[1,2] S. T. Cundiff,[2] Y. Aiura,[4] K. Oka,[4] H. Eisaki,[4] and D. S. Dessau[1,2,†]




Science **310**, 1271 (2005)



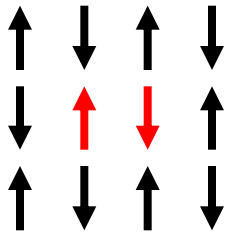

$$J = 146(4)\ \text{meV}$$

By fitting the spin wave dispersion measured by neutron scattering. (also needs a small ring exchange term.)

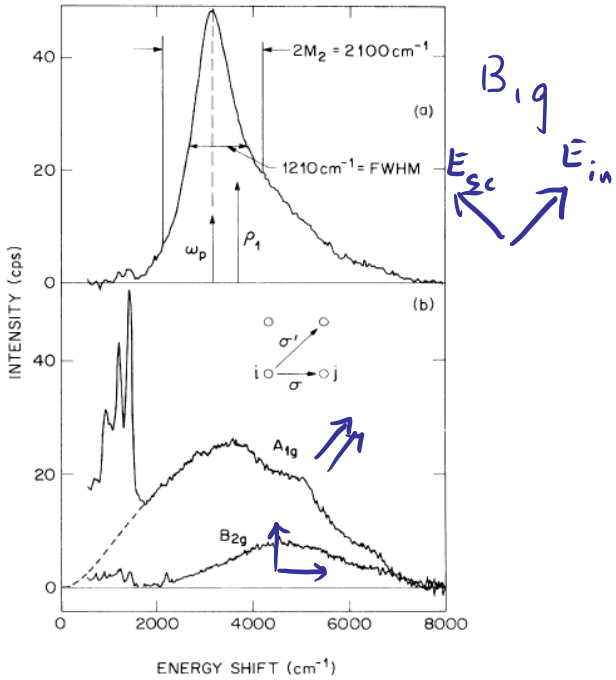
Also from Raman scattering.

$$I(\omega) = \sum_i \delta(\omega - (E_i - E_0)) \,|\langle 0 | H_R | i \rangle|^2$$

$$H_R = \sum_{\langle ij \rangle} (\mathbf{E}_{\text{inc}} \cdot \boldsymbol{\sigma}_{ij})(\mathbf{E}_{\text{sc}} \cdot \boldsymbol{\sigma}_{ij}) \mathbf{S}_i \cdot \mathbf{S}_j$$



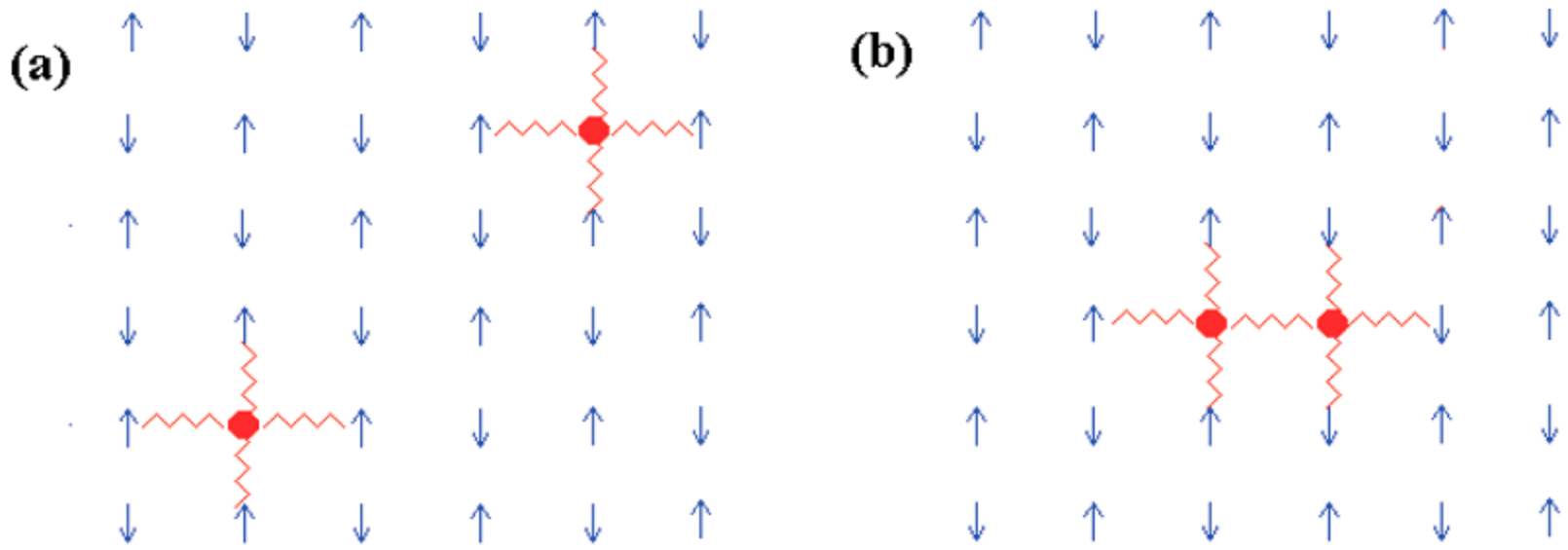
Spin flip breaks 6 bonds, costs 3J.




Largest J known among transition metal oxide, except for the Cu-O chain compound where J=220meV.

Adapted from Patrick Lee and T. Senthil

- **2-d hole-pairing:**
- AF-coupling causes holes to form pairs.




unpaired: 8 bonds broken

paired: 7 bonds broken