Lectures

Lect. 1	Introduction	Ch.1; 2.1-2.5; 8.9
Lect. 2	Interactions, environment	3.1, Ch.4; 7.1-7.7
Lect. 3	Ordering, Domains	5.1-5.3; 6.7; 8.3, 8.7, 8.8
Lect. 4	Symmetry breaking	6.1-6.6
Lect. 5	Quantum magnetism	8.1-8.6

Magnetism

Origin of magnetism

- Orbital magnetism (p -> p+eA)
- Spin magnetism (spin S, localized, itinerant)

Magnetic interactions

- Dipole
- Exchange interaction (direct, indirect)
- RKKY (itinerant exchange)
- Double exchange
- Anisotropic exchange (LS interaction)

Magnetism

Diamagnetism:

- No magnetic moments
- No magnetic interaction
- Response due to induced currents
- Magnetization opposite to field

Paramagnetism:

- Magnetic moments (spin, orbit)
- Weak magnetic interactions
- Response due to orientation
- Magnetization in field direction

Ordered magnetism:

- Magnetic moments
- Strong magnetic interactions
- Response due to polarization
- Ferro-, antiferro-, ferrimagnetic

‘Non-ordering magnetism’

Floating matter (magnetic levitation)

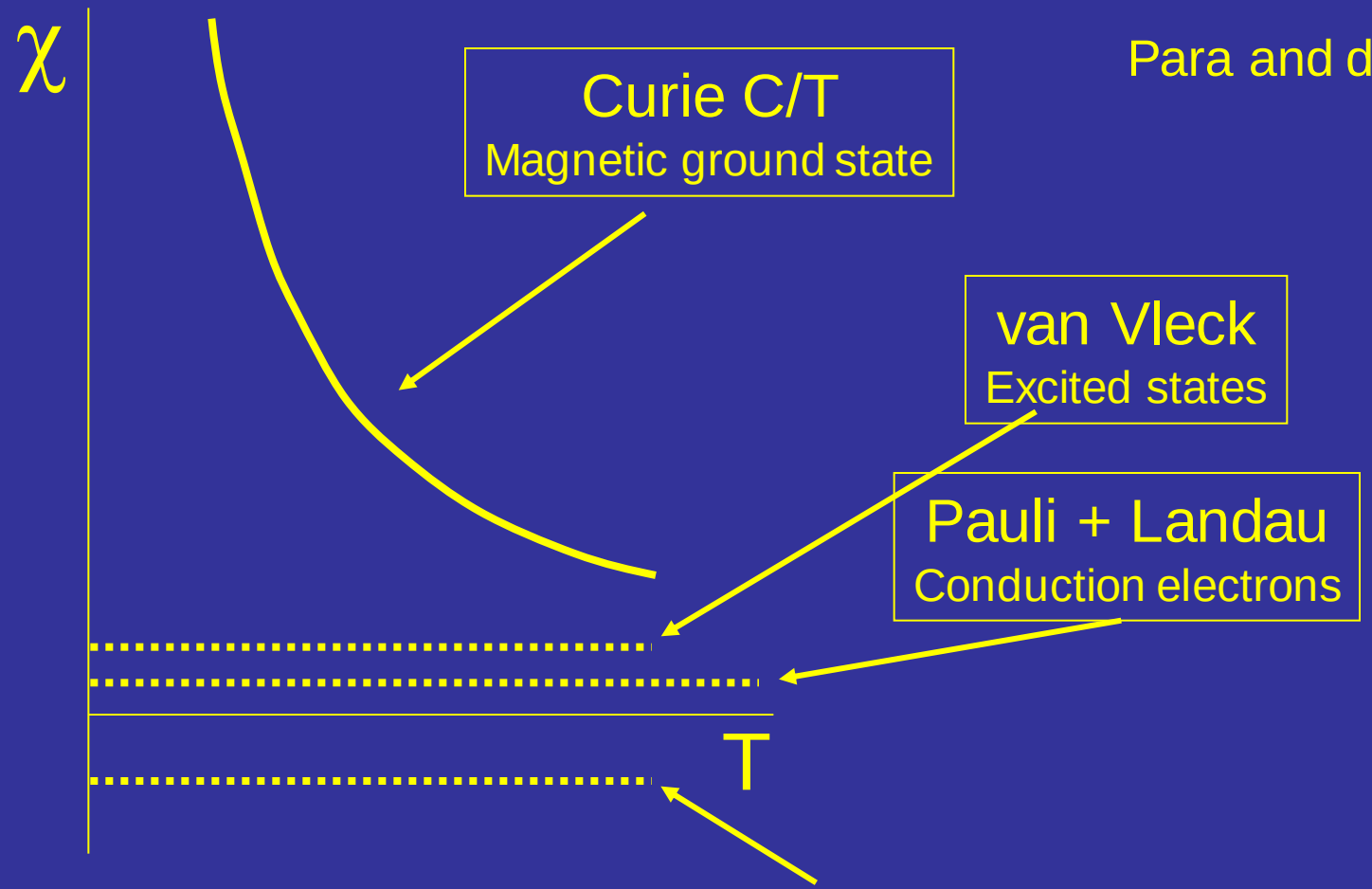
(perfect) diamagnetism

Floating $YBaCuO_{6+d}$

1986: J.G. Bednorz
& K.A. Mueller

Magnetism

Para and diamagnetism



$$M = \chi H$$

Magnetic moments

- Intrinsic magnetic moment of elementary particles: Spin
- Moving charges: Orbits

- Spin-orbit coupling ➔ J; m_J
- Magnetic moment:

$$\mu = g_J \sqrt{J \cdot (J+1)}\,\mu_B$$

$$\mu_z = g_J \cdot m_J \cdot \mu_B$$

- Energy in a field

$$E = g_J \cdot m_J \cdot \mu_B \cdot B$$

- Free electron spin (S=1/2) in 1 T:

$$\mu_s \approx 1.73\ \mu_B \qquad E \approx 60\ \mu\text{eV} \therefore 0.7\ \text{K}$$

Only orbits: $g_l=1$
Only electron spin: $g_s=2$
More general:

$$g_J = \frac{3J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

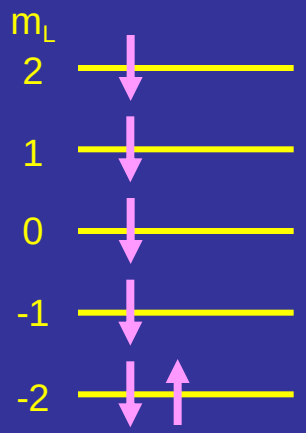
Bohr magneton

$$\mu_B = \frac{\hbar e}{2m_e} = 9.274\ \text{J/T} = 5.7883 \cdot 10^{-5}\ \text{eV/T}$$

Localized moments: partially filled shells

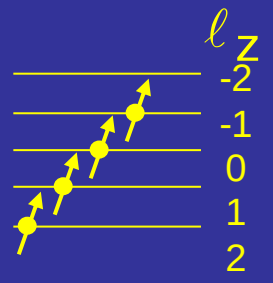
- d-levels, f-levels
- L-S coupling scheme
- Hund's rules
  1. **Maximize S** (→ spatially antisymmetric, decrease shielding)
  2. **Maximize L** (→ orbiting in same direction, decrease repulsion)
  3. **J=|L-S| for < half full**
     J=|L+S| for > half full (→minimize LS interaction)

example Fe^{2+}: $[Ar]3d^6$
6 electrons
Total spin: 2
Total L: 2
➔J=4
Term symbol ($^{(2s+1)}L_J$): $^5D_4$



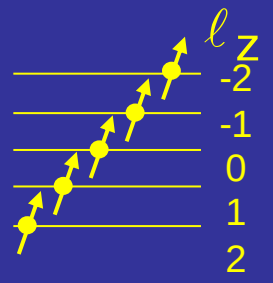
Some more examples

d-shell ($\ell = 2$), 4 electrons
Mn^{3+},Cr^{2+}



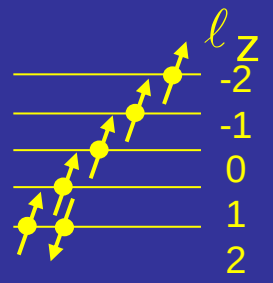
S=2
L=2 => $^5D_0$
J=0

d-shell ($\ell = 2$), 5 electrons
Fe^{3+},Mn^{2+}



S=5/2
L=0 => $^6S_{5/2}$
J=5/2

d-shell ($\ell = 2$), 6 electrons
Fe^{2+}



S=2
L=2 => $^5D_4$
J=4

Environment: crystal field

Rare earth's: 4f shell's small ('inner' electrons)
Iron group: 3d shell's on the outside

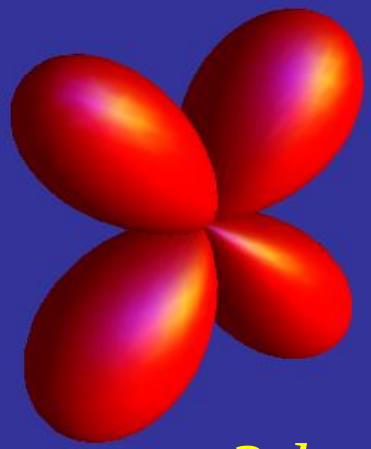
=> decoupling of L and S, J no longer good Quantum number
=> splitting of the 2L+1 orbital states
=> Quenching of the orbital angular momentum ($L_z \rightarrow 0$)

=> High spin – Low spin transitions
=> Jahn-Teller distortions
=> Orbital excitations (orbitons)

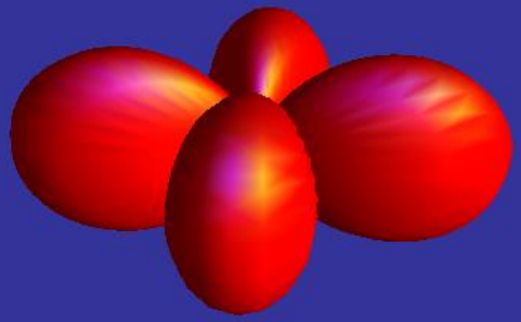
Anisotropy

Kramers degeneracy (local B-field probe)

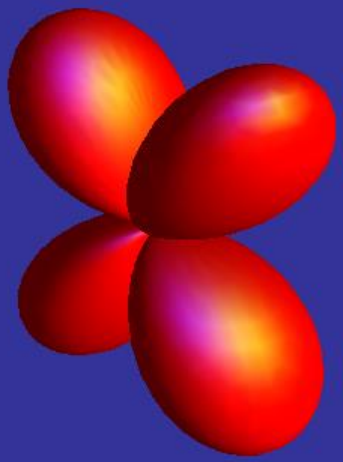
3d orbitals (Chem)



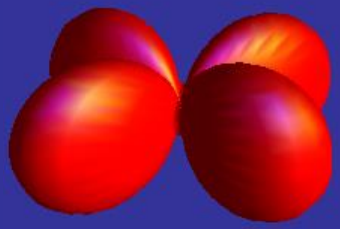
$3d_{xz}$



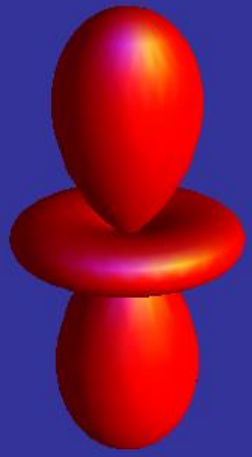
$3d_{xy}$



$3d_{yz}$

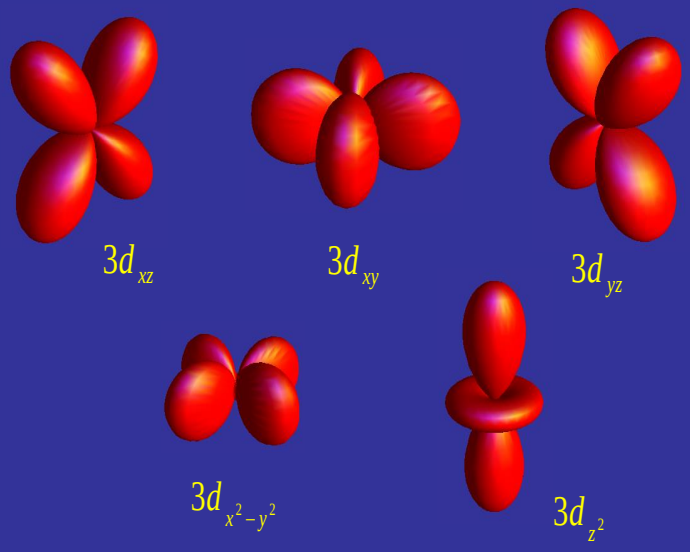


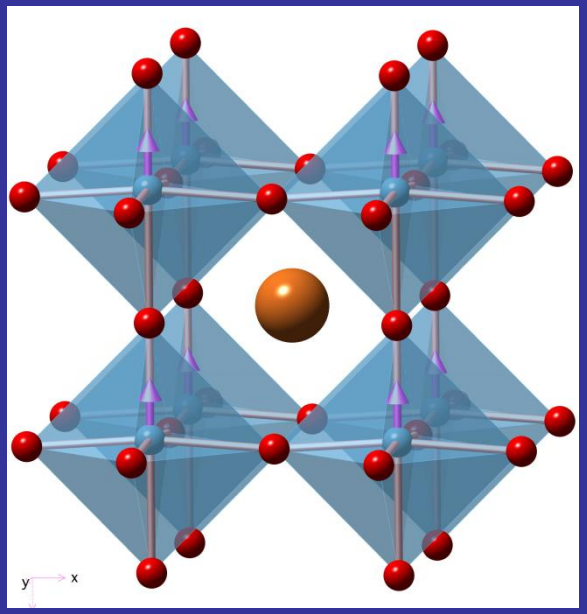
$3d_{x^2-y^2}$



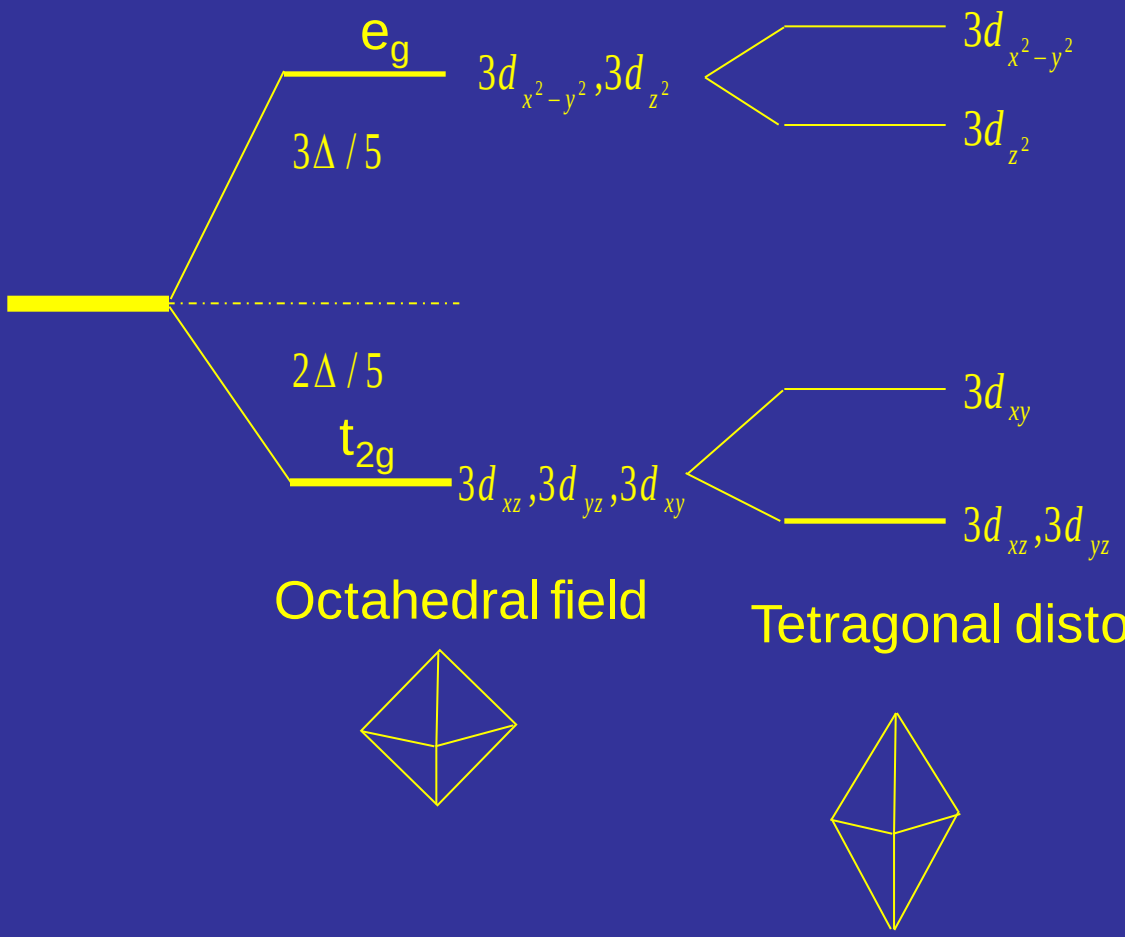
$3d_{z^2}$

3d orbitals in a CF





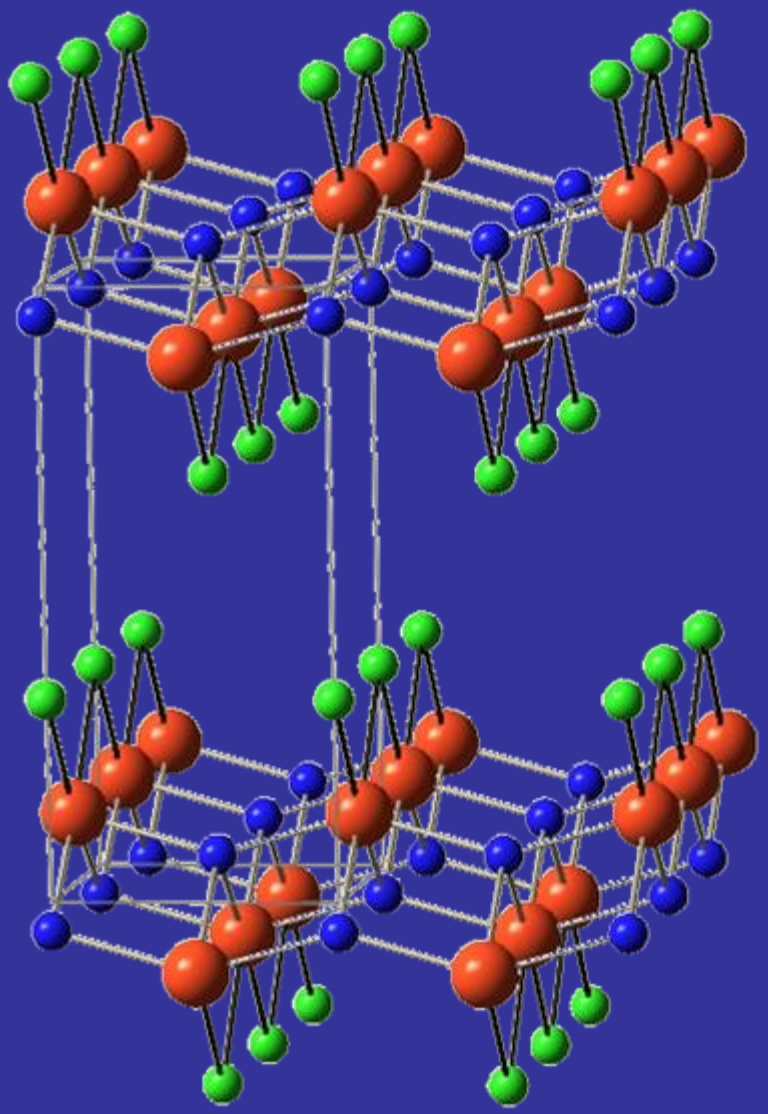
Perovskite structure (ABO_3 e.g. $BaTiO_3$)



Octahedral field

Tetragonal distortion

TiOX



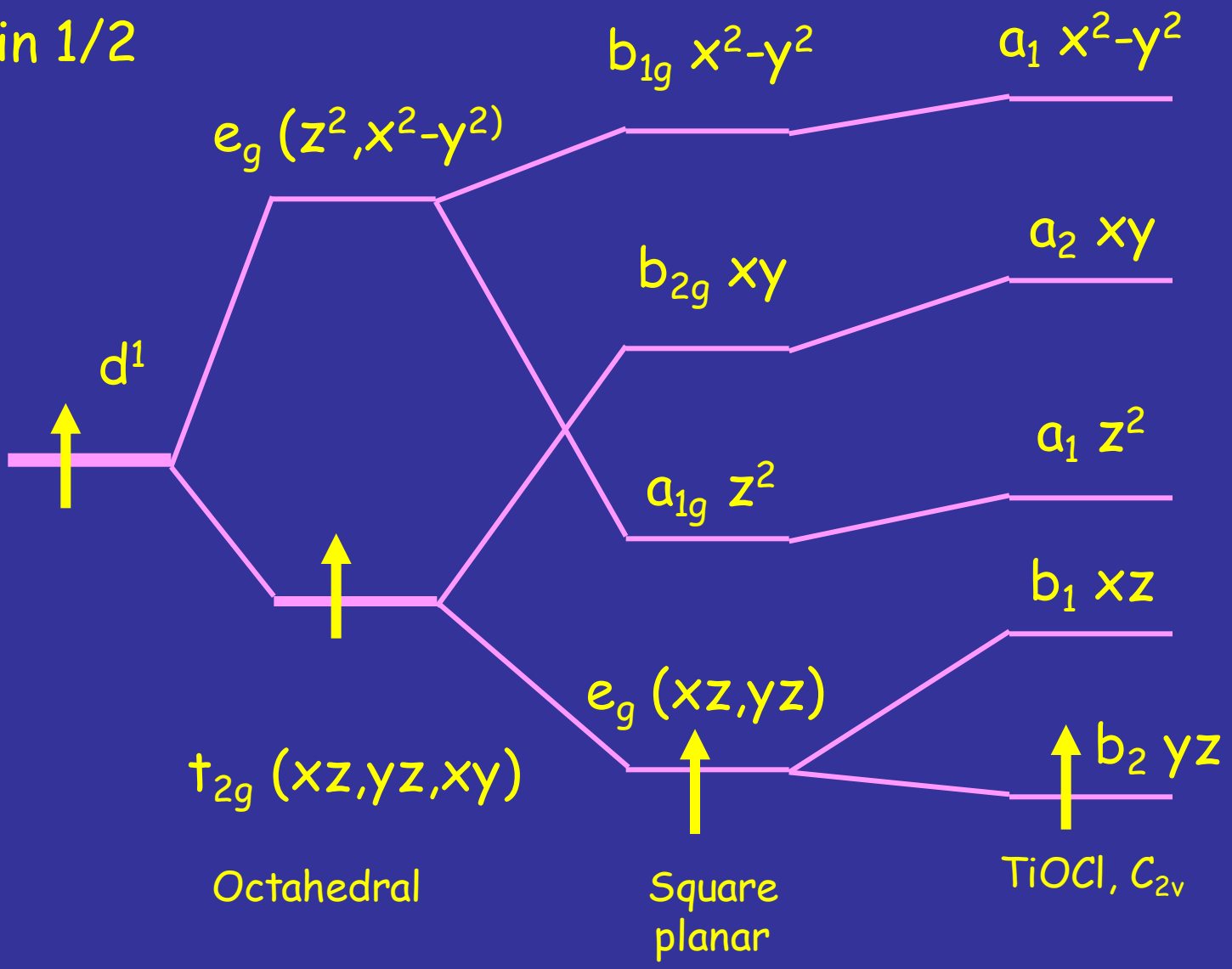
Pmmn

Double bi-layer of
TiO_4Cl_2 "Octaedra"

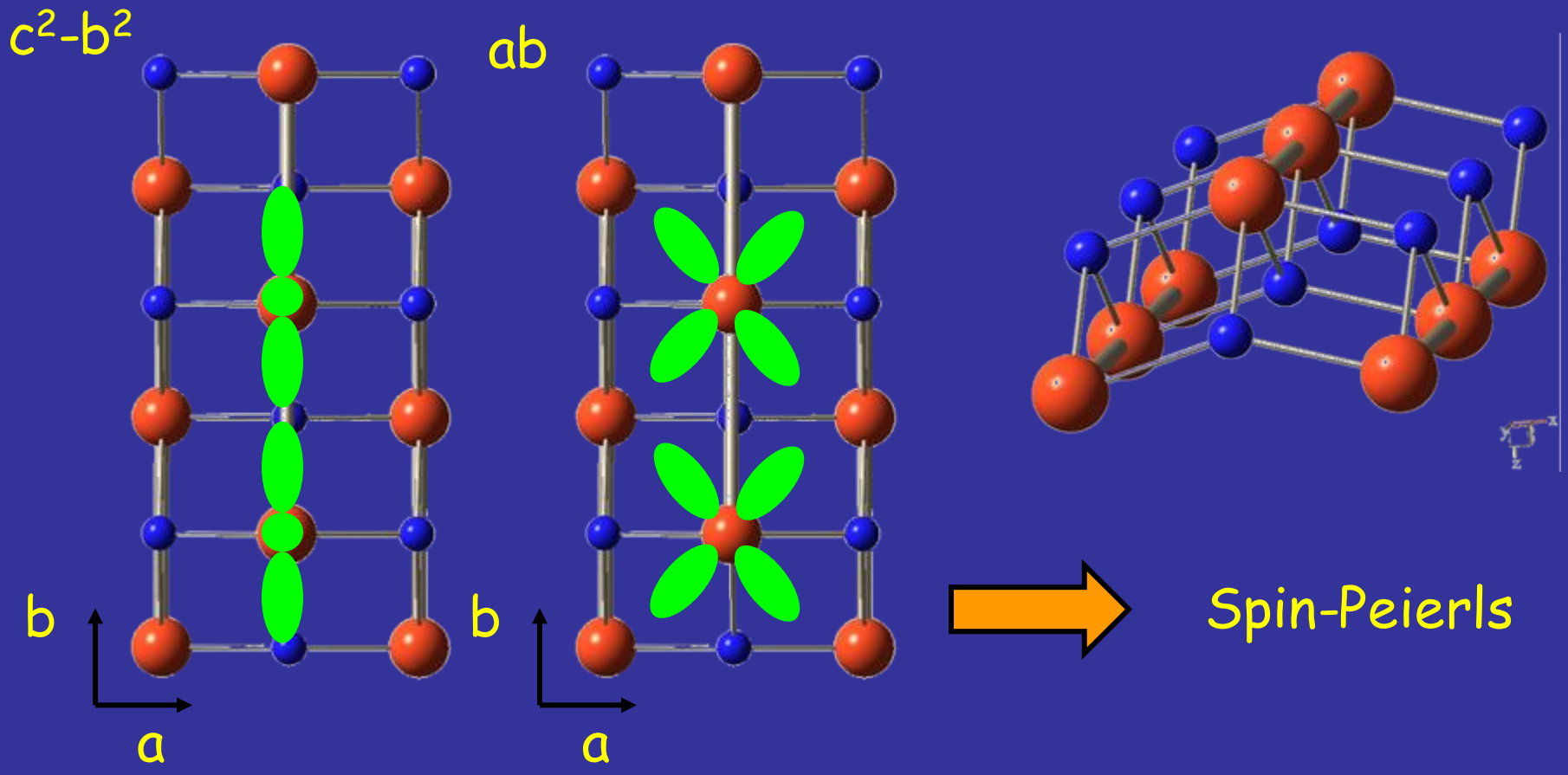
Layered:
Cl-Cl distance 3.7 Å

3d levels in TiOX

Ti^{+} $3d^1$, spin 1/2

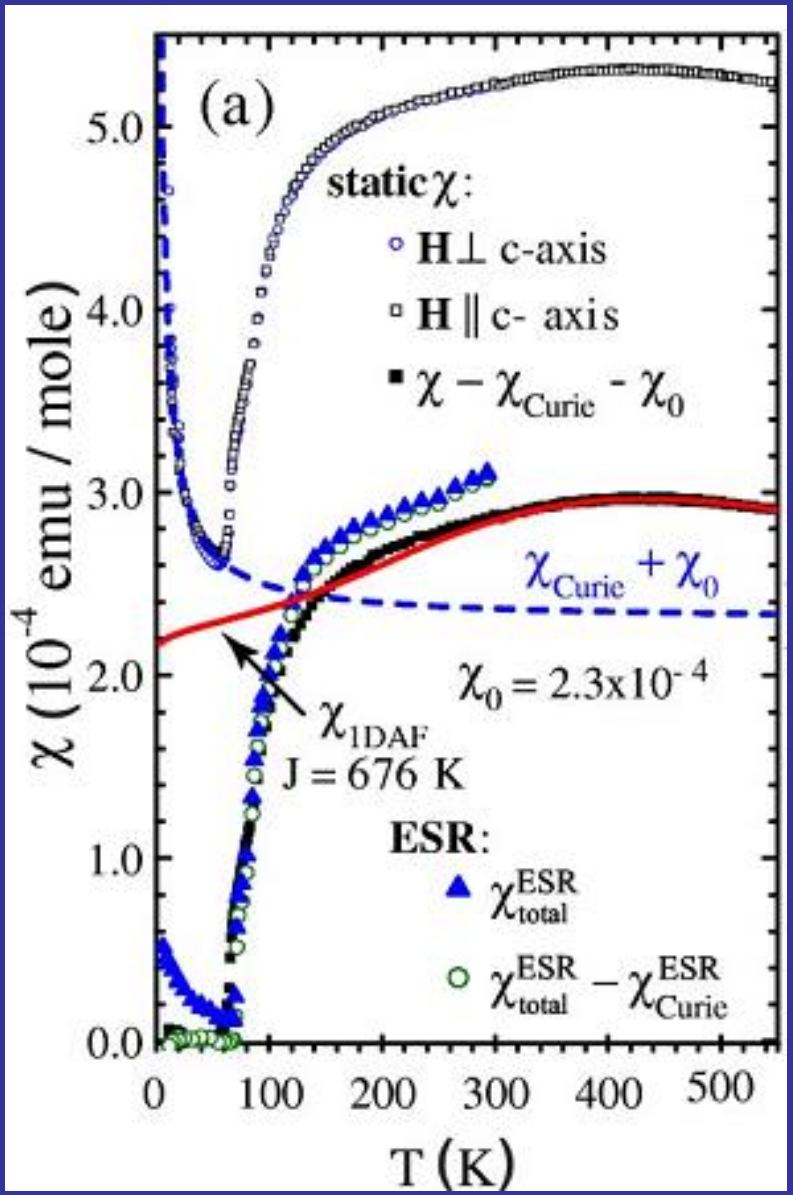


Occupied orbitals



Exchange through direct Ti-Ti interaction along b ➔ 1D system
Mott-Hubbard ➔ AF interaction

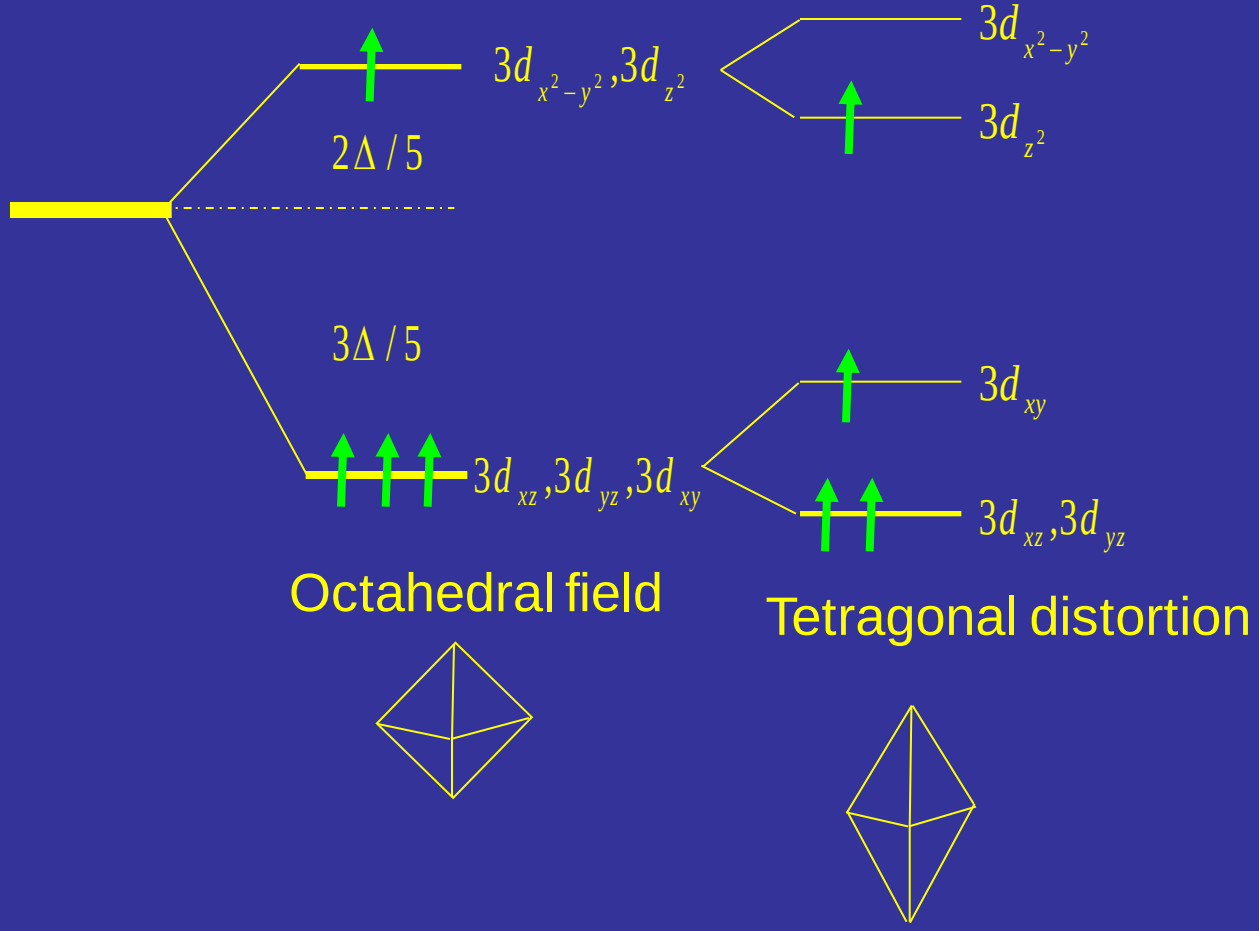
Susceptibility TiOX



Kataev et al., PRB 68, 140405 (2003)

Above T_c: Typical 1D Heisenberg AF
Below T_c: Opening of a gap due to dimerization

Jahn Teller distortion



Mn^{3+} : $3d^4$

Energy gain due to lowering e_g orbital

Cost: elastic energy

Strong e-p coupling

Does not work for Mn^{4+}

Jahn Teller effect

- Dynamic

  Fluctuations x,y,z distortions (e.g. cubic perovskites)

- Cooperative

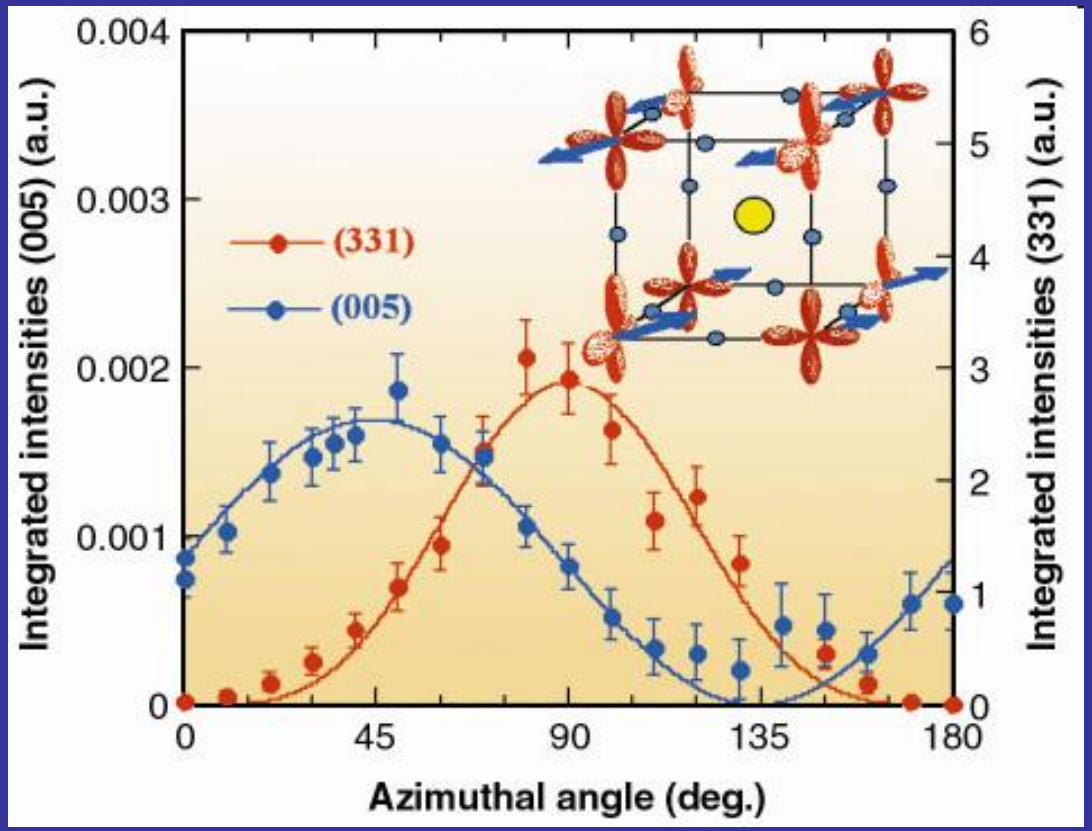
  Lattice mediated

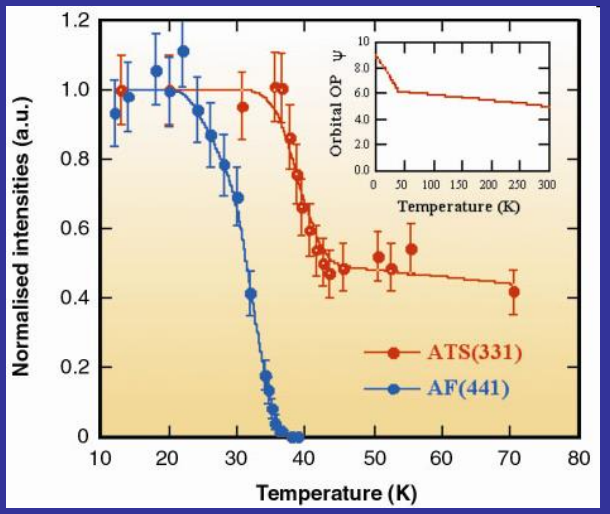
$LaMnO_3$: T > 800 K Cubic, below that tetragonal

$KCuF_3$: Orbital ordering (z^2-x^2 and z^2-y^2 orbitals)

Spin and Orbital ordering

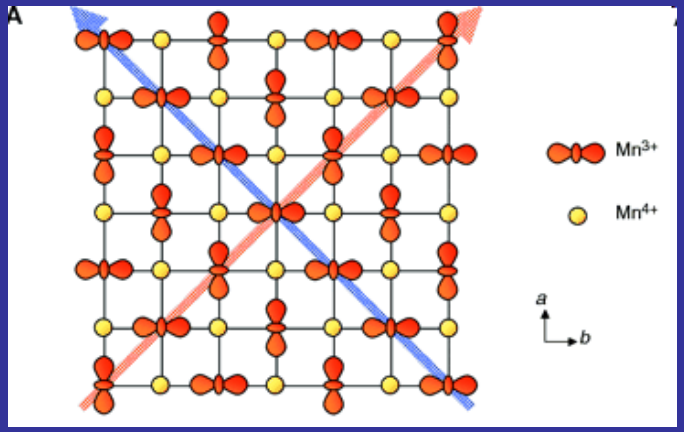
$KCuF_3$: Orbital ordering (z^2-x^2 and z^2-y^2 orbitals)





Murakami et al. PRL 1998

Charge and Orbital order



folk.uio.no/ravi

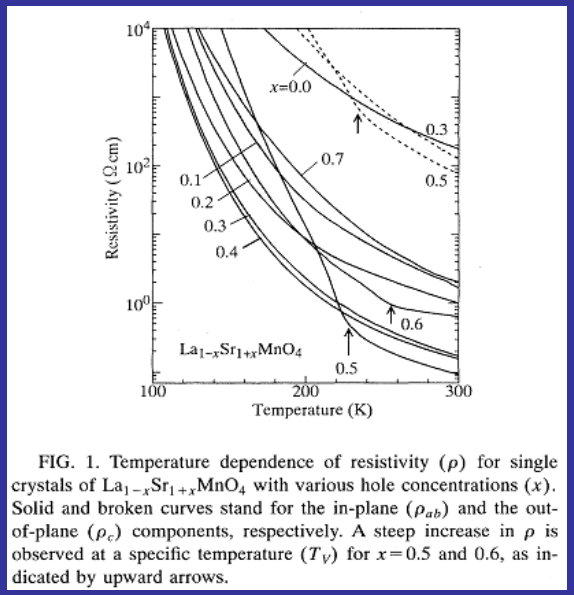


FIG. 1. Temperature dependence of resistivity (ρ) for single crystals of $La_{1-x}Sr_{1+x}MnO_4$ with various hole concentrations (x). Solid and broken curves stand for the in-plane (ρ_{ab}) and the out-of-plane (ρ_c) components, respectively. A steep increase in ρ is observed at a specific temperature (T_V) for $x=0.5$ and 0.6, as indicated by upward arrows.

Moritomo et al. PRB 1995

Charge, Orbital, Spin order in $La_{0.5}Sr_{1.5}MnO_4$

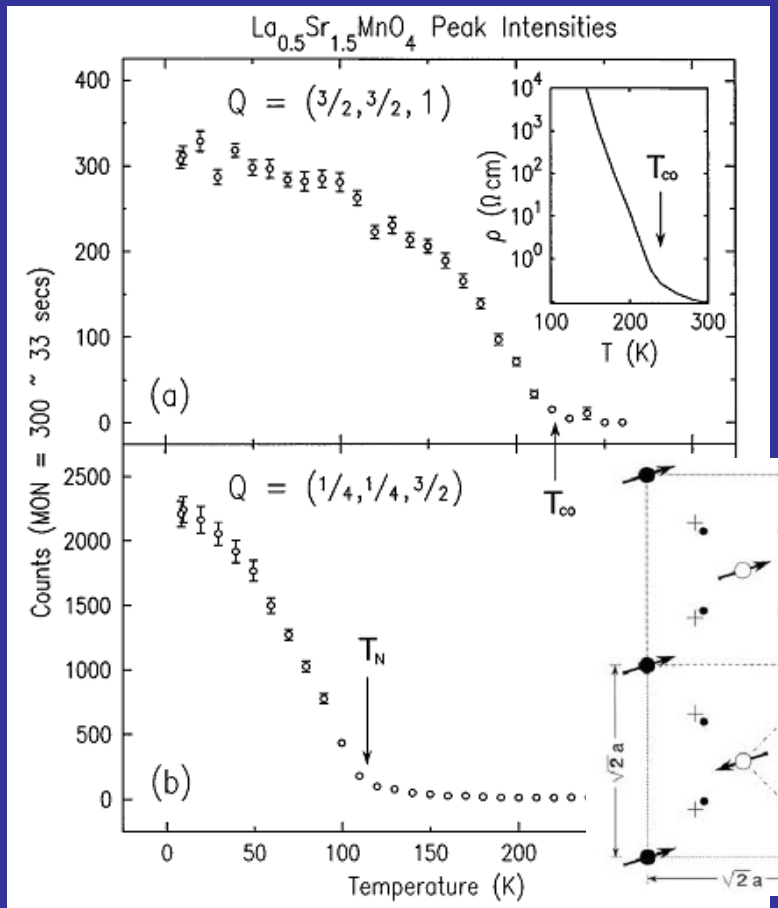


FIG. 4. Temperature dependence of the (a) charge and (b) magnetic order. Inset in (a): Resistivity vs T.

Sternlieb et al. PRL 1996