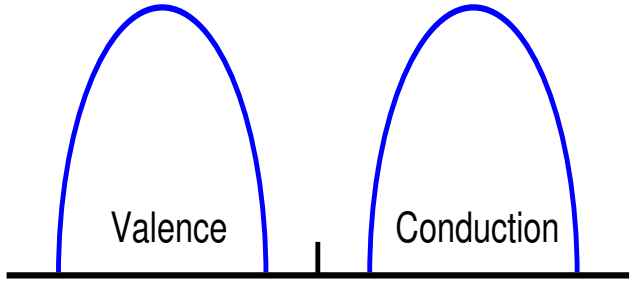
Hybrid Mott Band Metal Insulator Transitions

Ansgar Liebsch

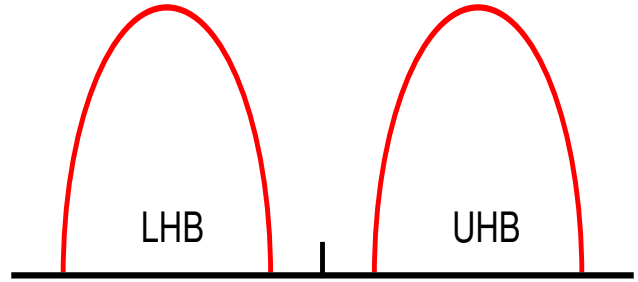
Institute for Solid State Physics

Research Center Jülich

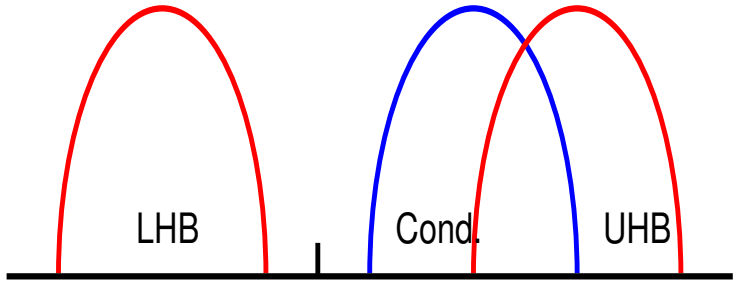
Band vs Mott Insulator → 'Hybrid Insulators'

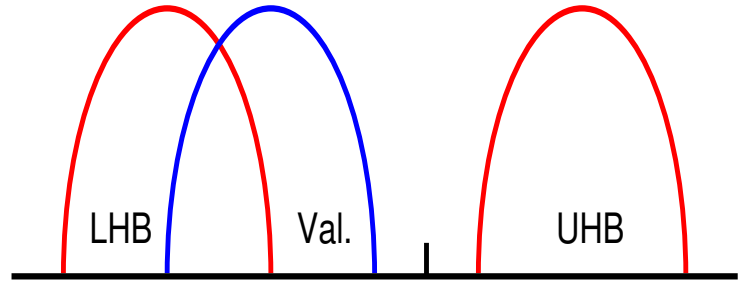


Band Insulator



Mott Insulator

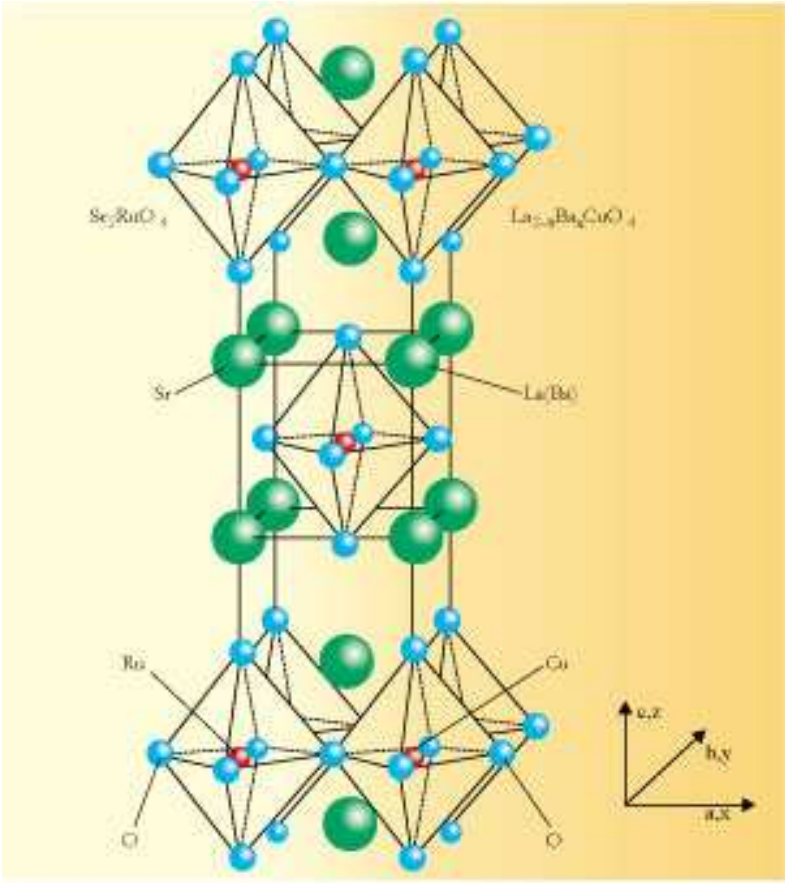


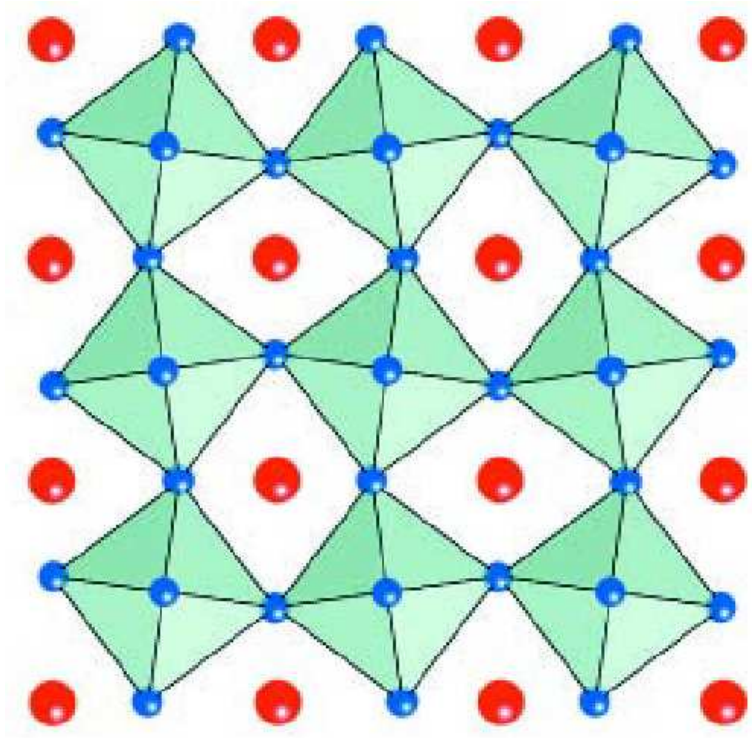


Overview

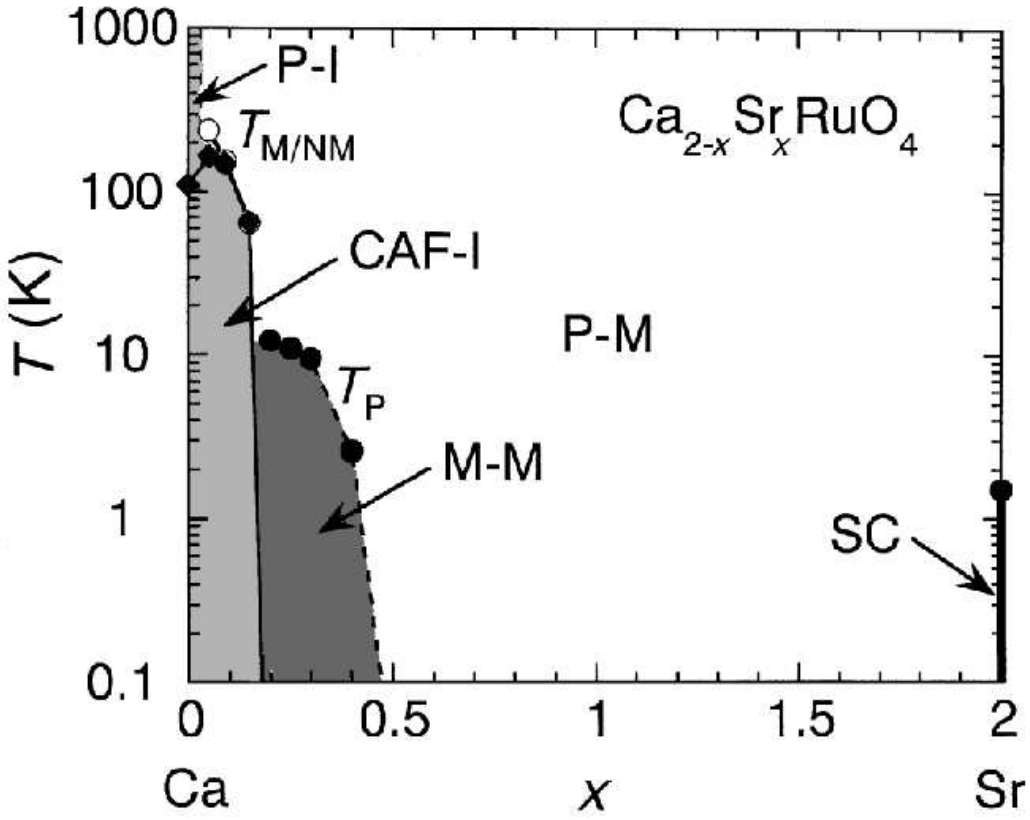
- Mott transition in multi-orbital materials:
  - Coulomb driven inter-orbital charge transfer
  - role of crystal field splitting
  - suppression of orbital fluctuations
  - subband filling / emptying $\rightarrow$ MIT
- Dynamical mean field theory:
  - exact diagonalization for multiband materials
- $Ca_{2-x}Sr_xRuO_4$ $4d^4$ orbital selective Mott transition ?
- V_2O_3 $3d^2$ Hund vs. Ising exchange ?
- $LaTiO_3$ / $SrTiO_3$ $3d^1$ MIT in heterostructures ?
  $3d^{1-x}$ doping driven Mott transition ?
- Na_xCoO_2 $3d^{5+x}$ topology of Fermi surface ?

Transition metal oxides: $Ca_{2-x}Sr_xRuO_4$



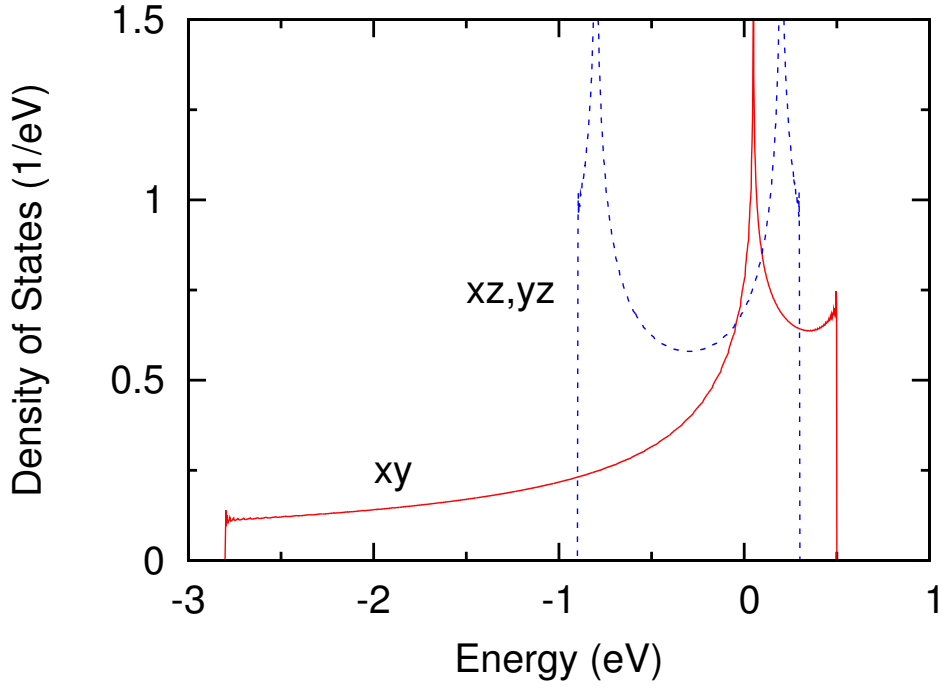


$Ca_{2-x}Sr_xRuO_4$: phase diagram



Maeno (PRL 2000)

$Ca_{2-x}Sr_xRuO_4$:



- coexisting narrow and wide bands: U/W_i ??
- orbital selective Mott transitions ? (Anisimov et al)
- crystal field splitting among t_{2g} bands ! (Fang et al)
- Sr $\rightarrow$ Ca: octahedral distortions

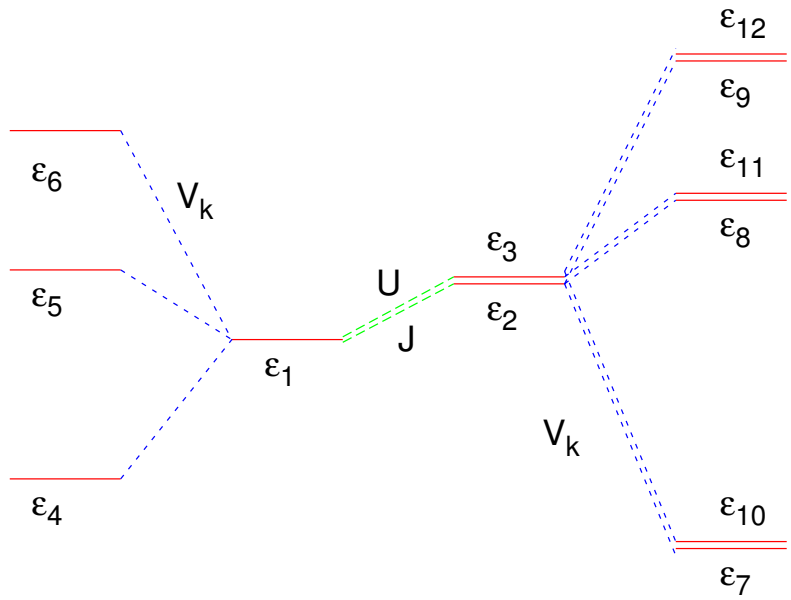
Dynamical mean field theory

$$G(i\omega_n) = \sum_k \Big(i\omega_n + \mu - H(k) - \Sigma(i\omega_n) \Big)^{-1}_{ij} \qquad (t_{2g})$$

$$G_0 = (G^{-1} + \Sigma)^{-1}$$

exact diagonalization: solid $\longrightarrow$ cluster = impurity + bath

$$G_{0,i}(i\omega_n) \approx G^{cl}_{0,i}(i\omega_n) = \Big(i\omega_n + \mu - \varepsilon_i - \sum_{k=4}^{n_s} \frac{|V_{ik}|^2}{i\omega_n - \varepsilon_k} \Big)^{-1}$$



cluster Hamiltonian

$$H^{cl} = \sum_{i\sigma}(\varepsilon_i - \mu)n_{i\sigma} + \sum_{k\sigma}\varepsilon_k n_{k\sigma} + \sum_{ik\sigma} V_{ik}[c^+_{i\sigma}c_{k\sigma} + \text{H.c.}]$$
$$+ \sum_i U n_{i\uparrow}n_{i\downarrow} + \sum_{i<j\sigma\leq\sigma'}(U' - J\delta_{\sigma\sigma'})n_{i\sigma}n_{j\sigma'} - \sum_{i\neq j} J[\, c^+_{i\uparrow}c_{i\downarrow}c^+_{j'\downarrow}c_{j\uparrow} + c^+_{i\uparrow}c^+_{i\downarrow}c_{j\uparrow}c_{j\downarrow}]$$

cluster Green's function:

$$G^{cl}_i(i\omega_n) = \frac{1}{Z}\sum_{\nu\mu}\frac{|\langle\mu|c^+_{i\sigma}|\nu\rangle|^2}{E_\nu - E_\mu - i\omega_n}[e^{-\beta E_\nu} + e^{-\beta E_\mu}]$$
$$= \frac{1}{Z}\sum_\nu e^{-\beta E_\nu}\left(\sum_\mu \frac{|\langle\mu|c^+_{i\sigma}|\nu\rangle|^2}{(E_\nu - E_\mu) - i\omega_n} + \sum_\mu \frac{|\langle\mu|c_{i\sigma}|\nu\rangle|^2}{(E_\mu - E_\nu) - i\omega_n}\right)$$

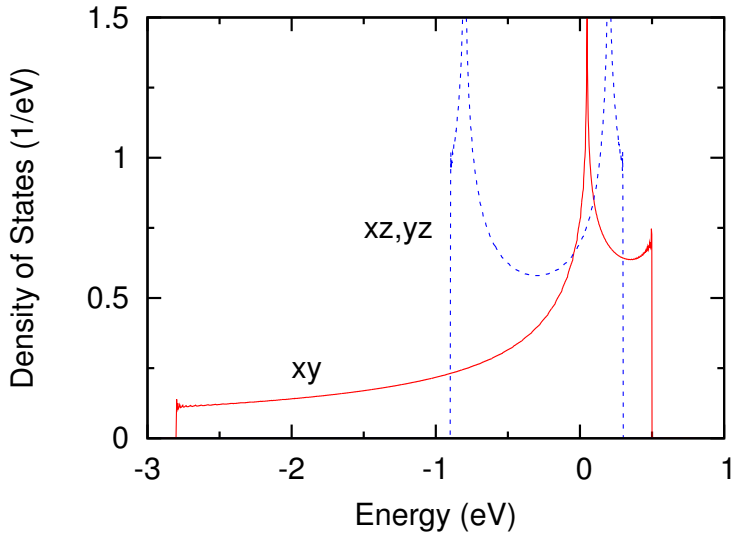
assumption: cluster self-energy $\approx$ solid self-energy:

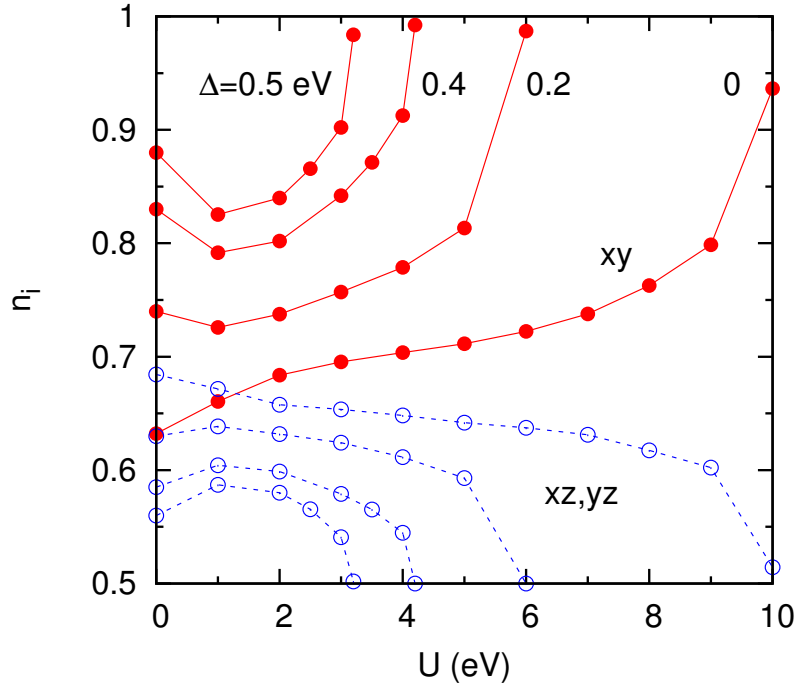
$$\Sigma^{cl} = 1/G^{cl}_0 - 1/G^{cl} \approx \Sigma$$

H^{cl} sparse: Arnoldi algorithm $n_s = 12$ $N = 853776$
level spacing $<$ 1 meV $\rightarrow$ finite size effects reduced
ED/DMFT for realistic t_{2g} materials, Hund exchange
complementary to QMC/DMFT Perroni, Ishida + A.L. PRB (2007)

$Ca_{2-x}Sr_xRuO_4$ nature of Mott transition ?

Sr $\rightarrow$ Ca : n_{xy} increases : crystal field Δ Fang et al (2004)





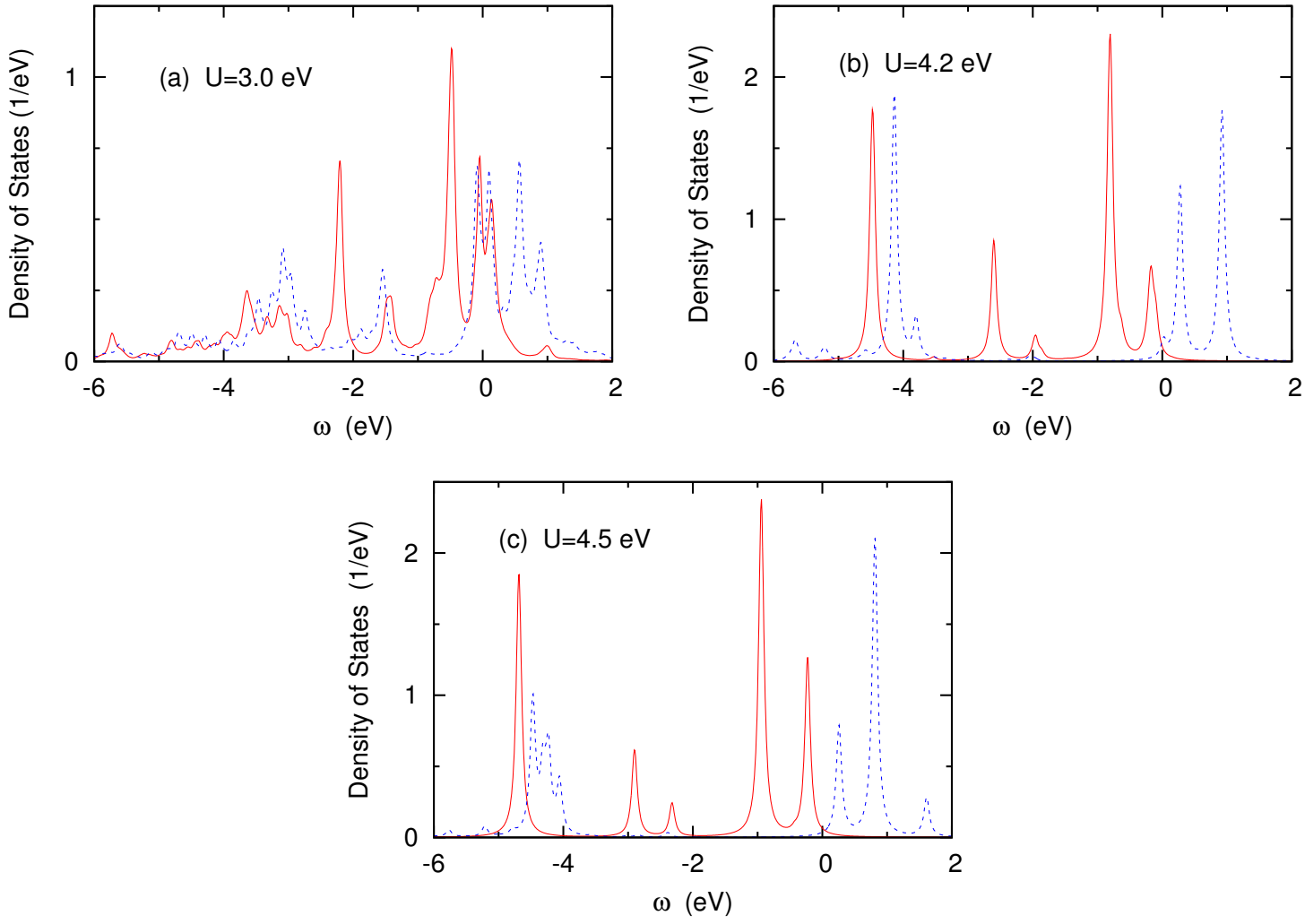
dyn. correl.: $n_{xy} \rightarrow 1$ A.L.+ Ishida, cond-mat/0612539 PRL(2007)

suppression of orbital fluctuations:

MIT in half-filled xz,yz band $\rightarrow$ no orbital selective MIT

future: role of octahedral distortions ? magnetic phases ?

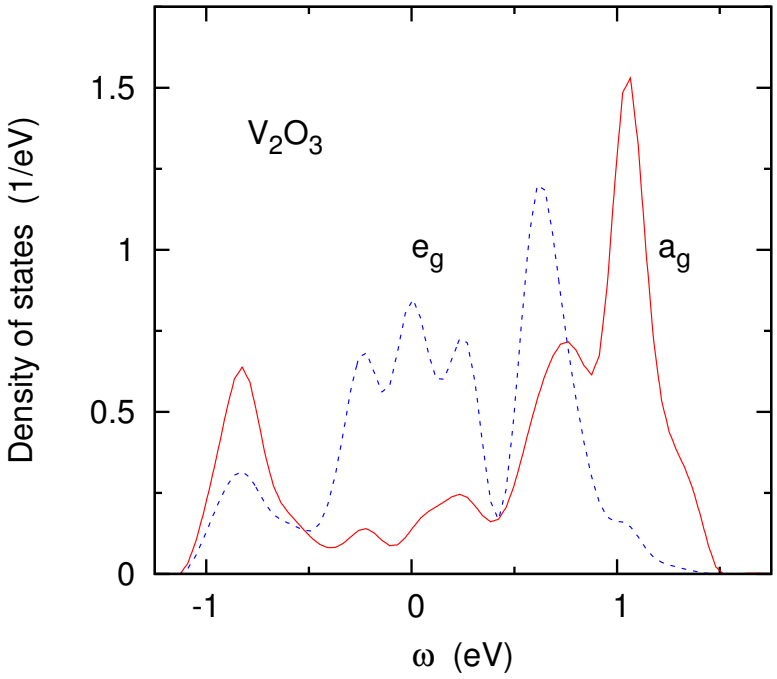
Ca_2RuO_4 cluster spectra $\Delta = 0.4$ eV



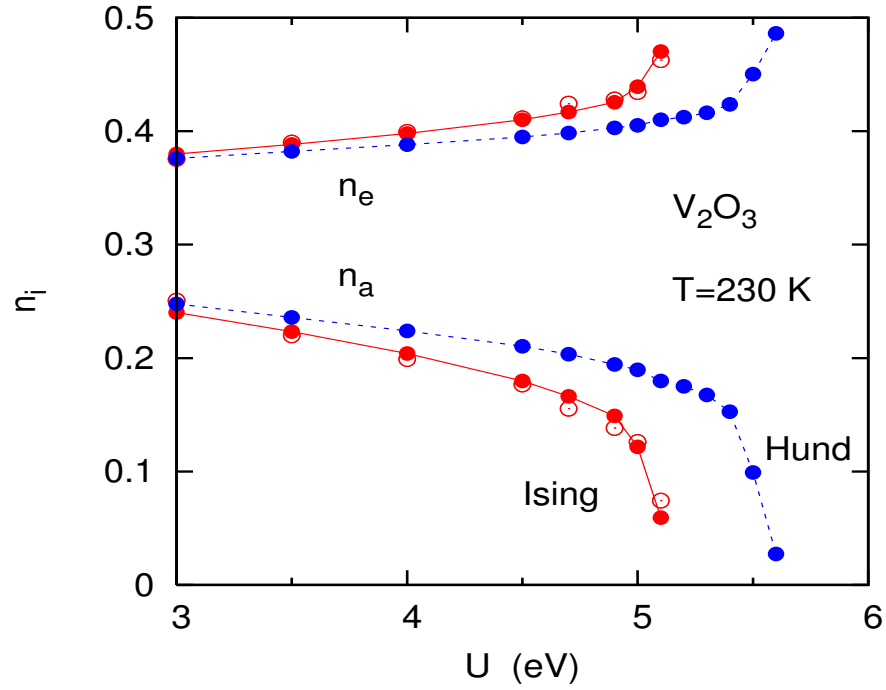
gap between filled xy and xz,yz upper Hubbard band

V_2O_3 $3d^2$

ED vs QMC



Keller et al, PRB (2004)

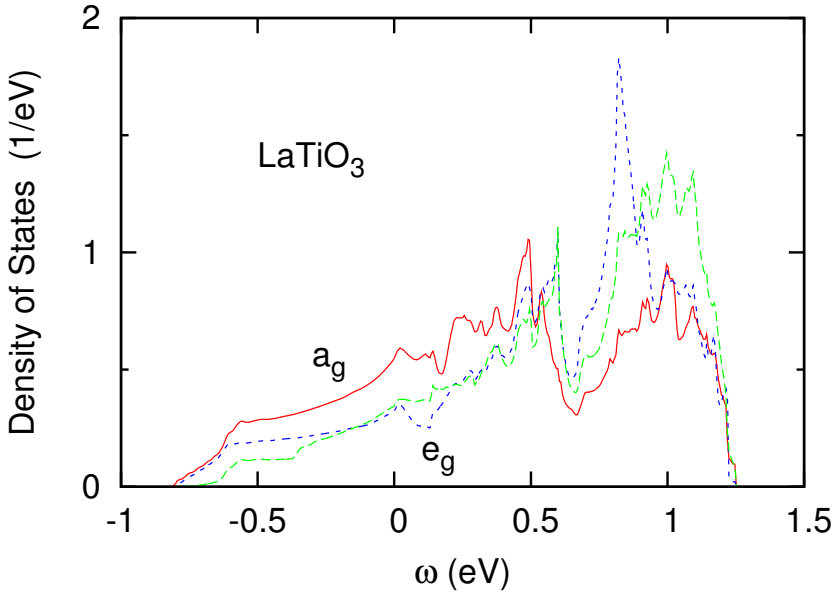


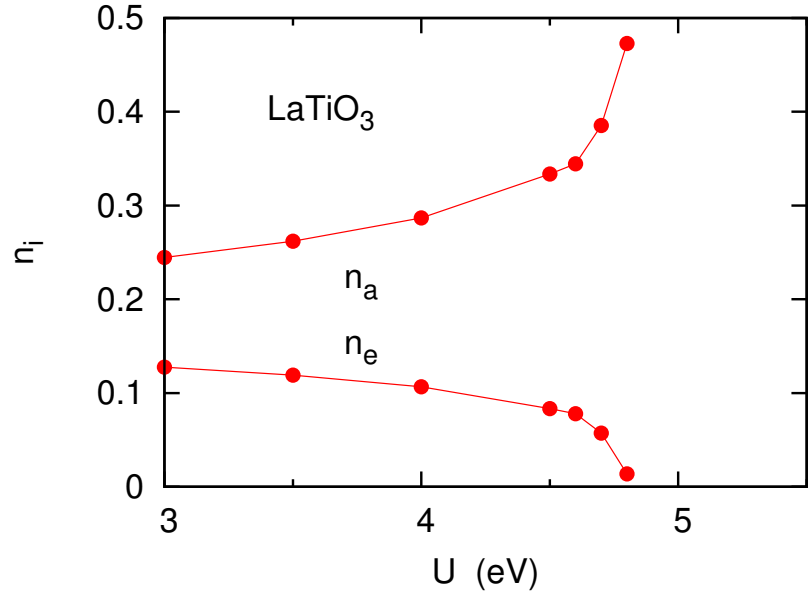
A.L. (2007)

dynamical correlations: $n_{a_g} \to 0$, MIT in half-filled e'_g

suppression of orbital fluctuations

$LaTiO_3$ $3d^1$



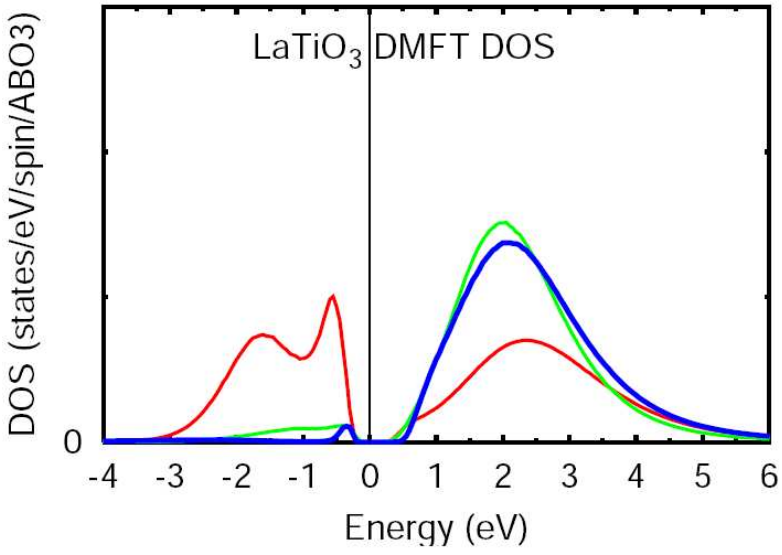


Pavarini et al, PRL (2004)

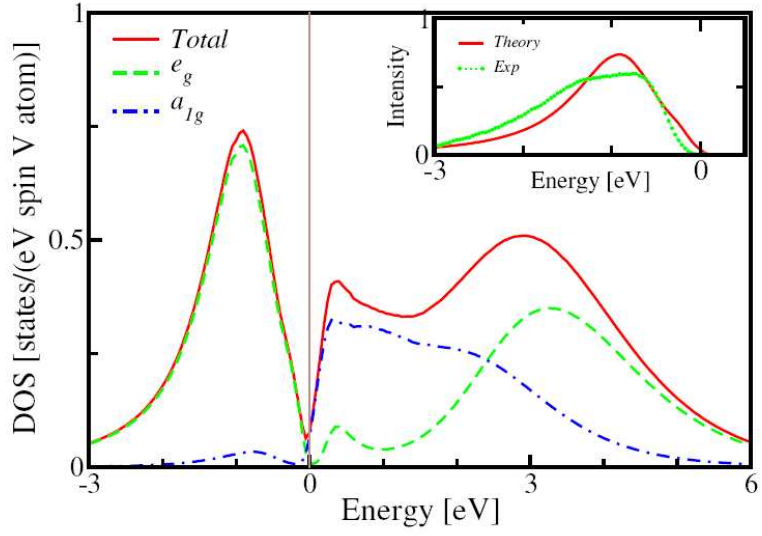
A.L. (2007)

dynamical correlations: $n_e \to 0$, MIT in half-filled a_g
suppression of orbital fluctuations

quasi-particle spectra: $LaTiO_3$ V_2O_3



Pavarini et al (2006)



Poteryaev et al, cond-mat/0701263

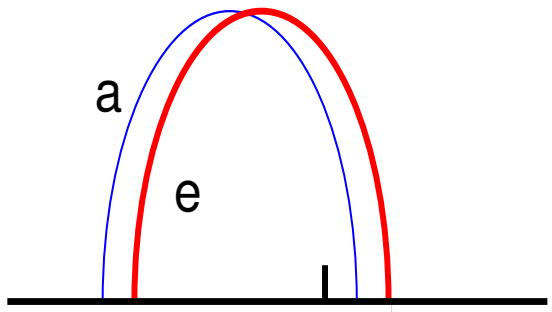
excitation gap:

$LaTiO_3$: LHB a_g $\rightarrow$ empty e_g bands

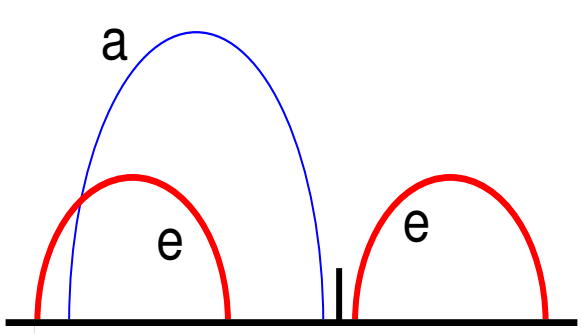
V_2O_3: LHB e_g $\rightarrow$ empty a_g band

Ca_2RuO_4

$n_\sigma \approx (0.8, 0.6, 0.6)$
$\rightarrow (1.0, 0.5, 0.5)$

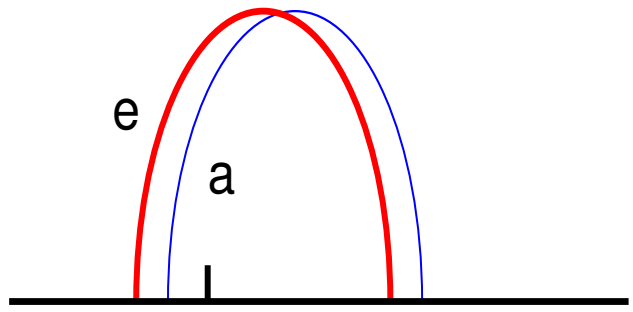


n=4

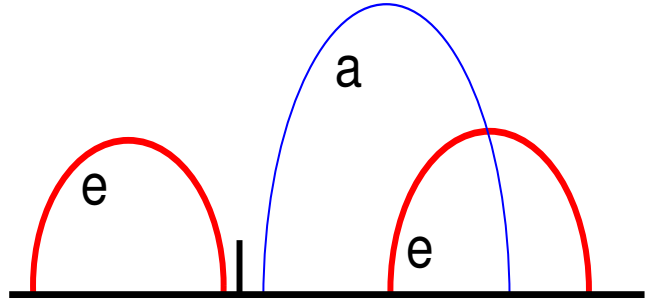


V_2O_3

$n_\sigma \approx (0.2, 0.4, 0.4)$
$\rightarrow (0.0, 0.5, 0.5)$

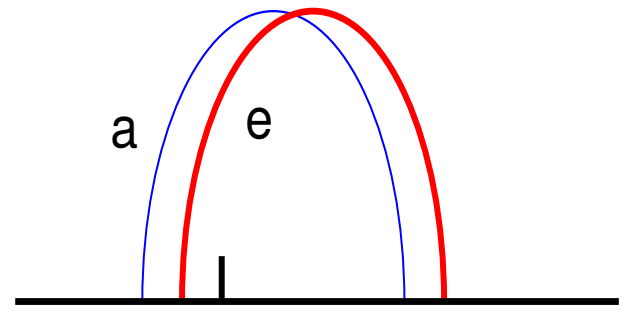


n=2

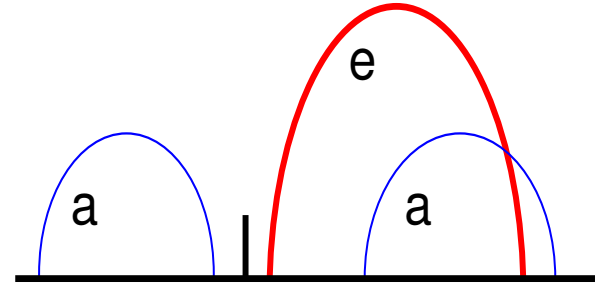


$LaTiO_3$

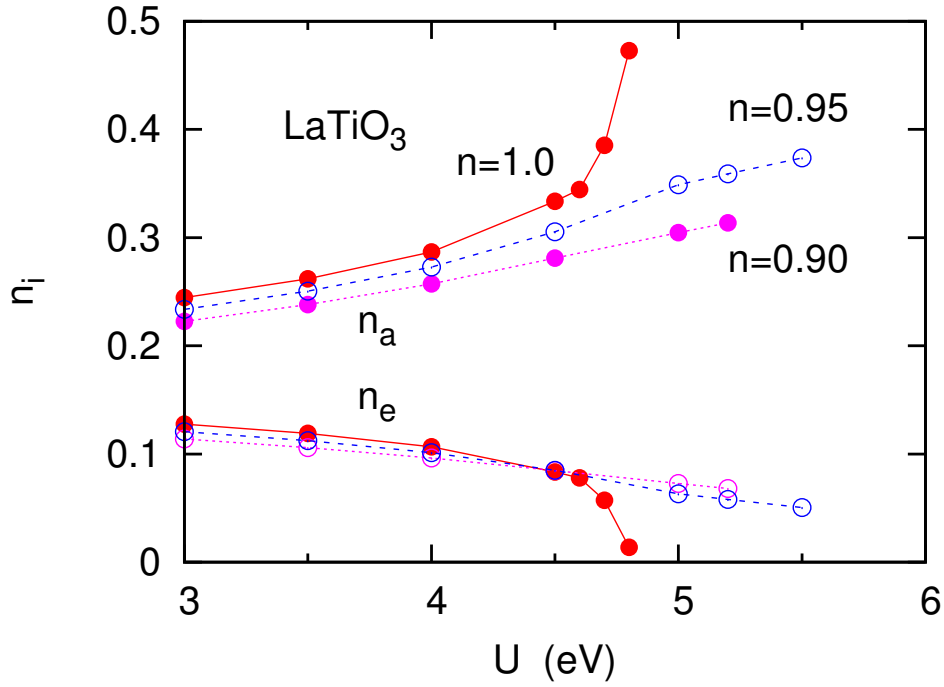
$n_\sigma \approx (0.3, 0.1, 0.1)$
$\rightarrow (0.5, 0.0, 0.0)$



n=1



$La_{1-x}Sr_xTiO_3$ $3d^{1-x}$ doping driven MIT



A.L. (2007)

$LaTiO_3$ / $SrTiO_3$ heterostructures: La / Sr interdiffusion:

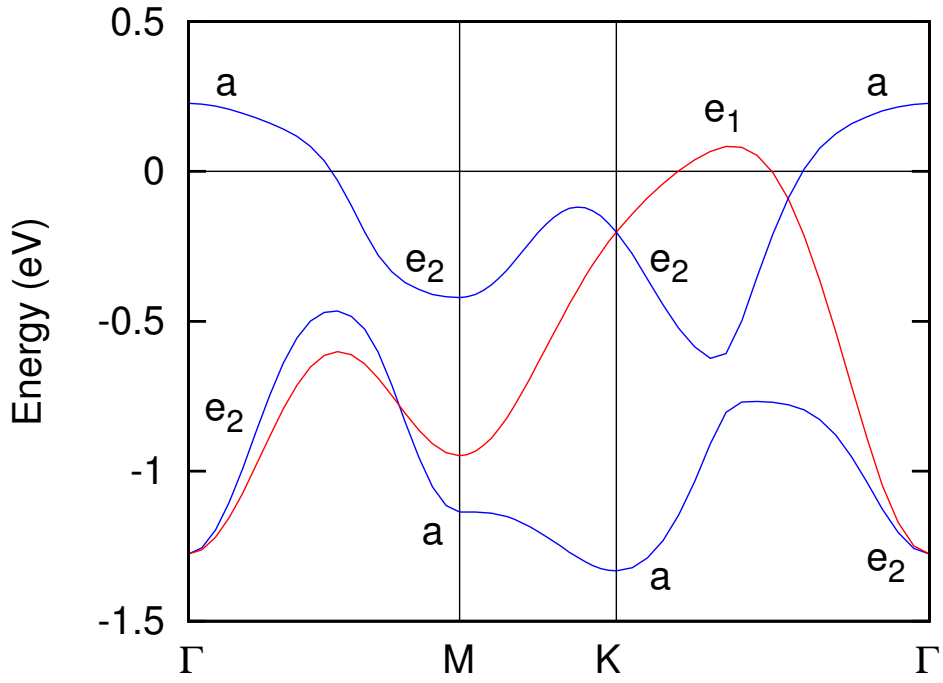
$3d^{0.95}$ inhibits $e_g \rightarrow a_g$ charge transfer: no MIT

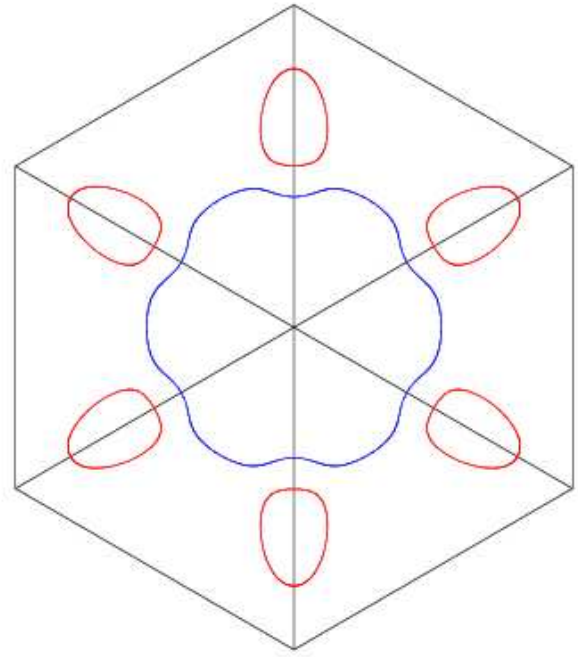
thin $LaTiO_3$ layers on $SrTiO_3$:

cubic symmetry shifts U_c upwards $\rightarrow$ no MIT at U_{Ti}

$Na_{0.3}CoO_2$: topology of Fermi surface ?

t_{2g} bands 0.4 a_g holes 0.3 e'_g holes D.J. Singh, PRB (2000)

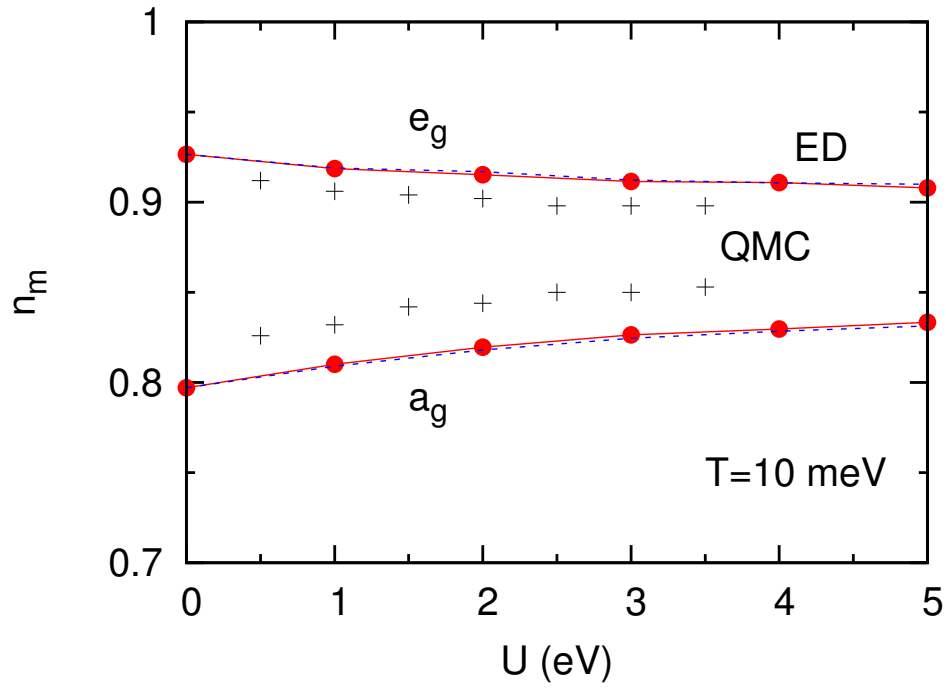




e_1 hole pockets not seen in ARPES ??

$Na_{0.3}CoO_2$ QMC vs ED / DMFT

Coulomb driven inter-orbital charge transfer for $J = U/4$

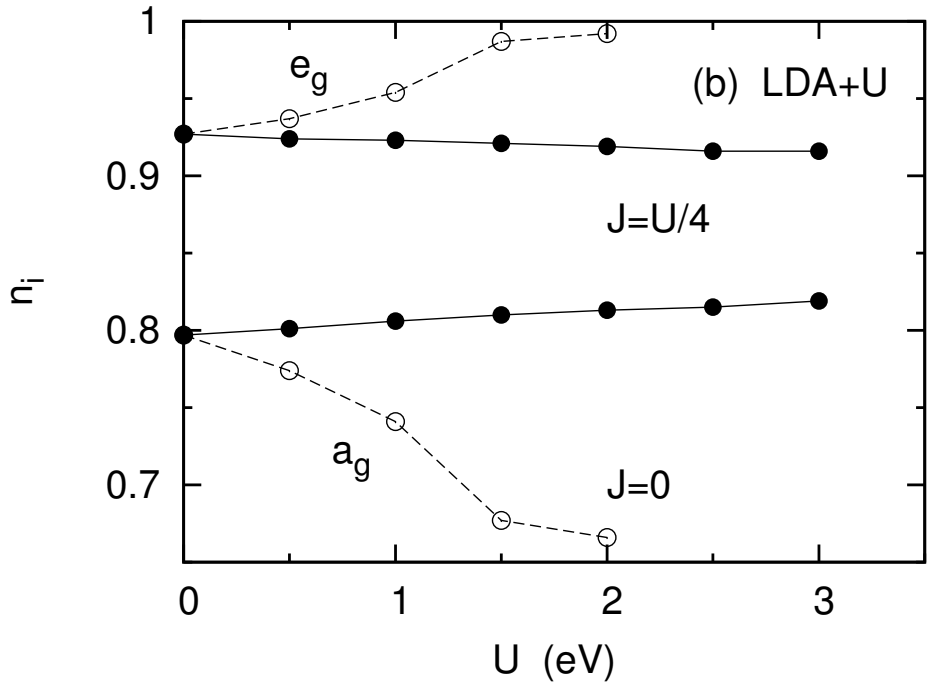


dynamical correlations: stabilization of e_g hole pockets

QMC: Ishida, Johannes + A.L. PRL (2005)

ED: Perroni, Ishida + A.L. PRB (2007)

$Na_{0.3}CoO_2$ LDA + U



Ishida, Johannes + A.L. PRL (2005)

$\Delta\epsilon_a = \ 2/3(n_e - n_a)(U - 5J)$

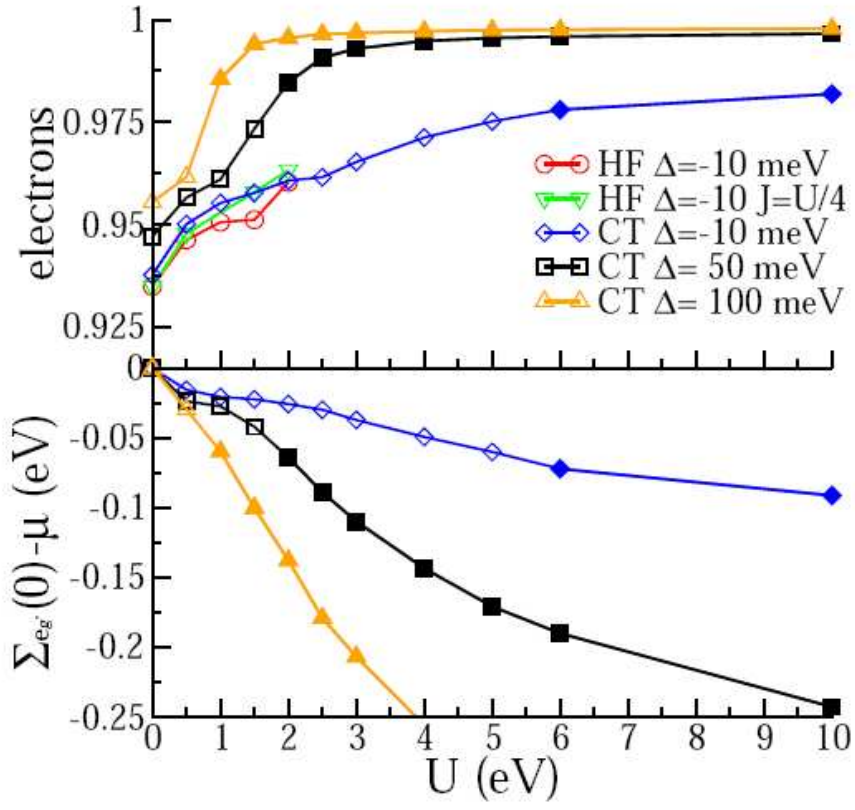
$\Delta\epsilon_e = -1/3(n_e - n_a)(U - 5J) \ \rightarrow$ J=0.9 eV: U_c=4.5 eV

subtle balance:

J vs U, shape of DOS, dynamical vs static correlations

$Na_{0.3}CoO_2$ QMC + crystal field

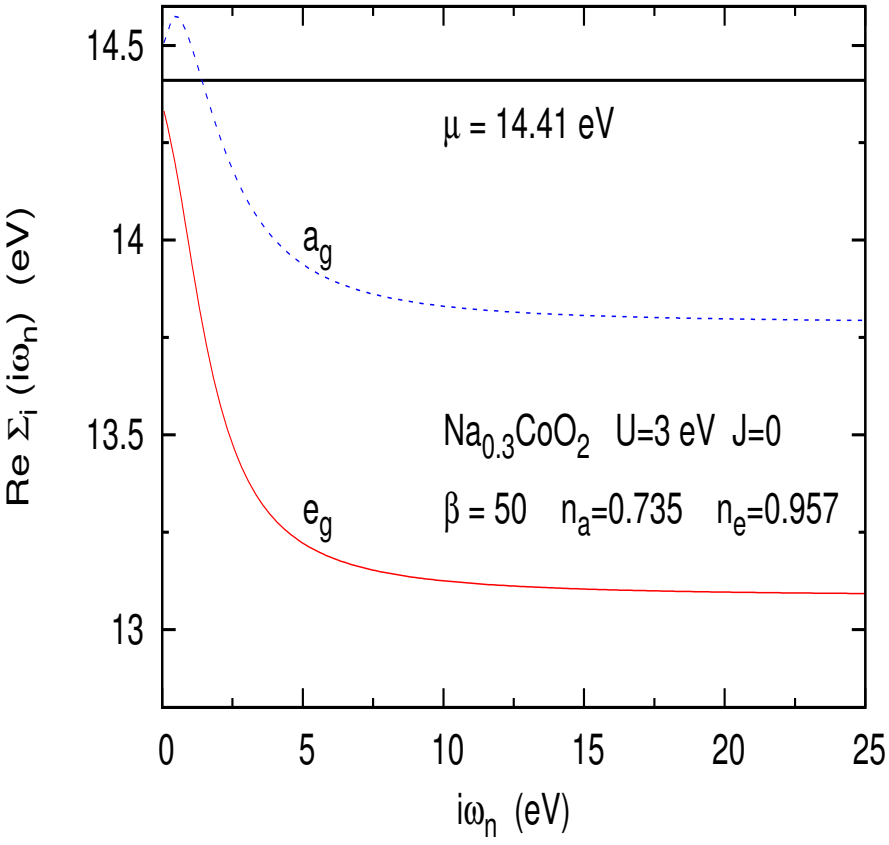
$\Delta = \epsilon_a - \epsilon_e$: e_g bands shifted down J=0



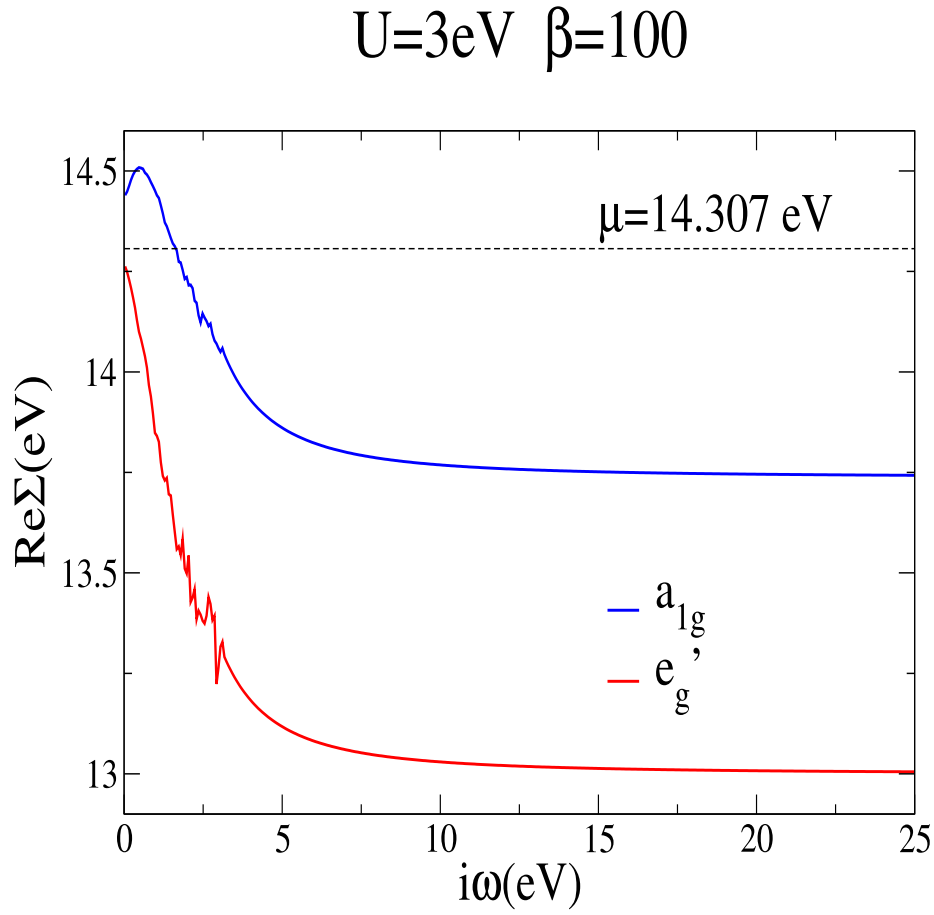
role of H(k) !

Marianetti, Haule, Kotliar, cond-mat/0612606

$Na_{0.3}CoO_2$ ED vs QMC same H(k)

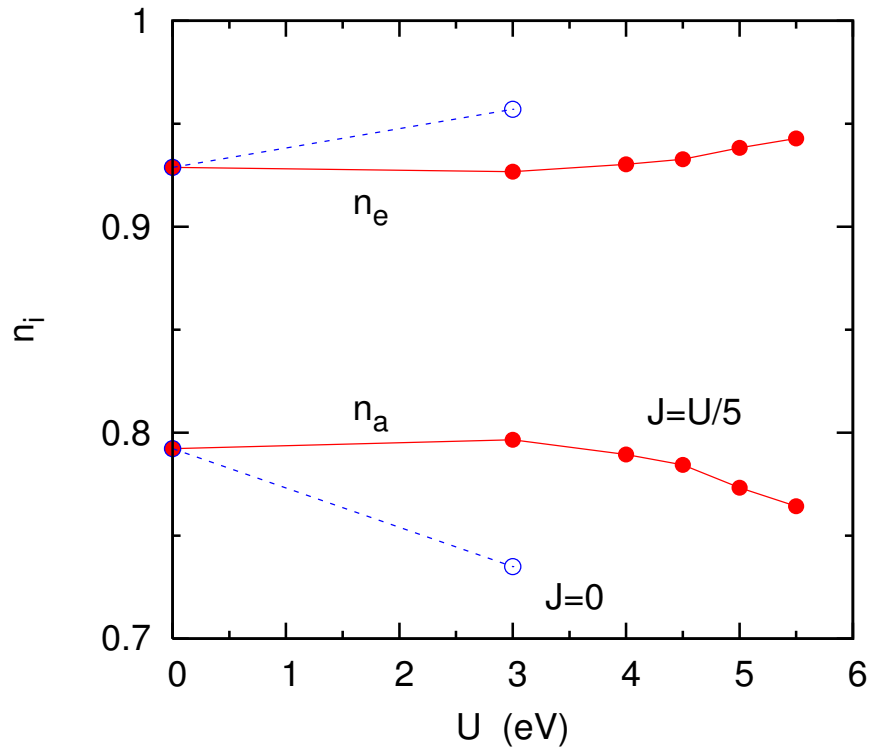


A.L. (2007)



Marianetti, Haule, Kotliar, cond-mat/0612606

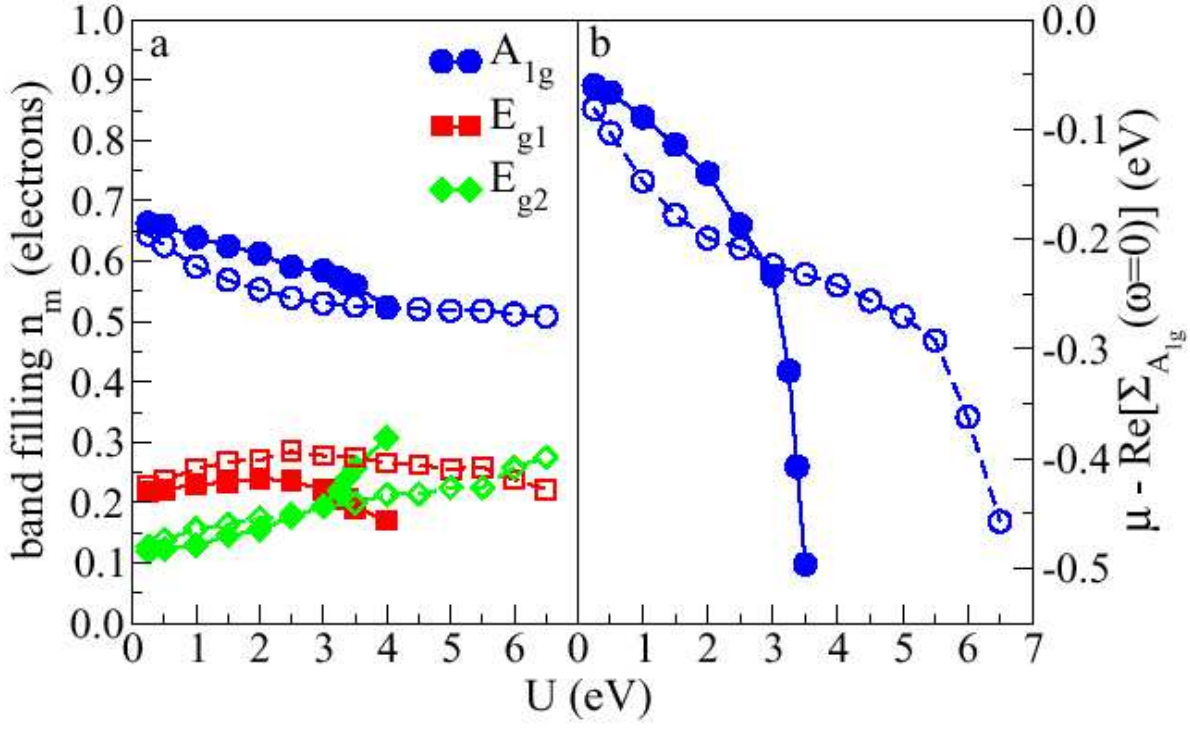
$Na_{0.3}CoO_2$ ED



H(k) Zhou et al, PRL (2005)

A.L. (2007)

$BaVS_3$

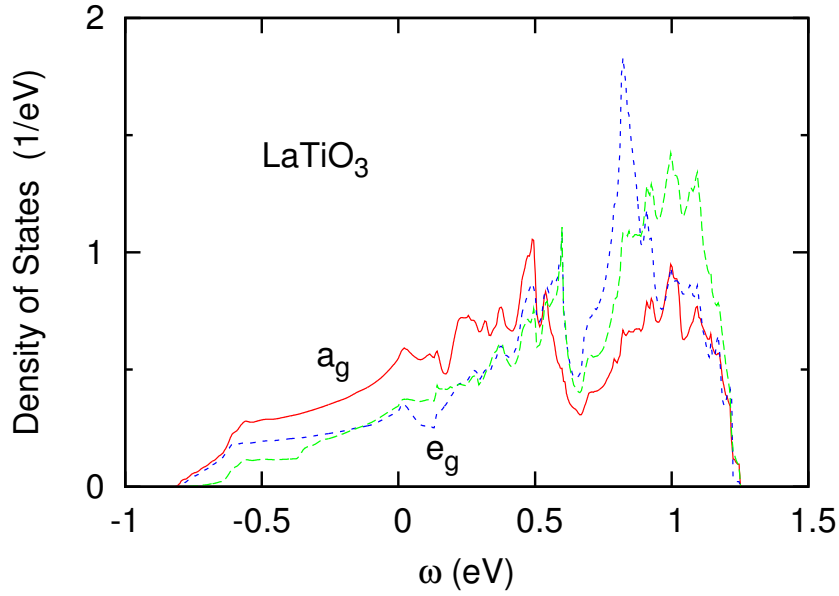


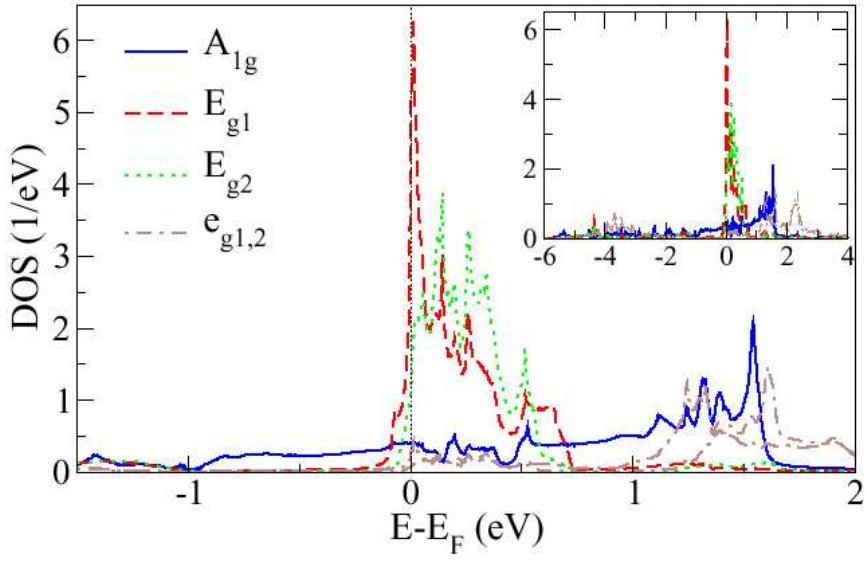
$J = U/4$ vs $J = U/7$

Lechermann et al, PRL (2005)

local Coulomb correlations can reduce / enhance orbital fluctuations !

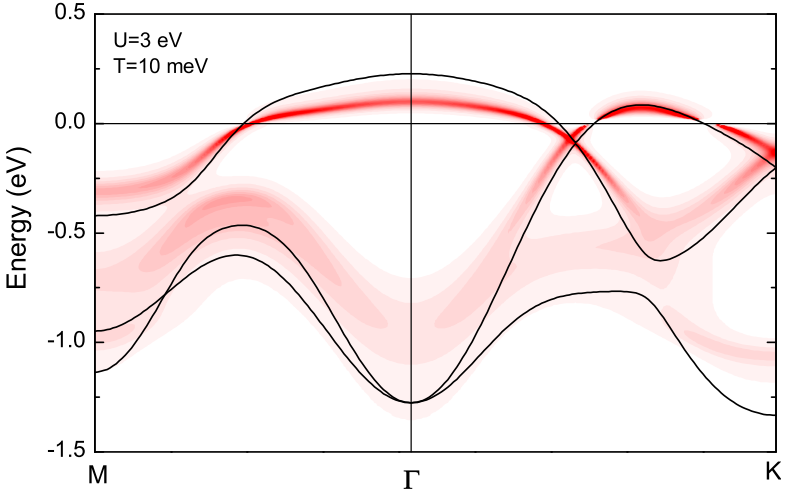
$LaTiO_3$ vs $BaVS_3$: both $3d^1$

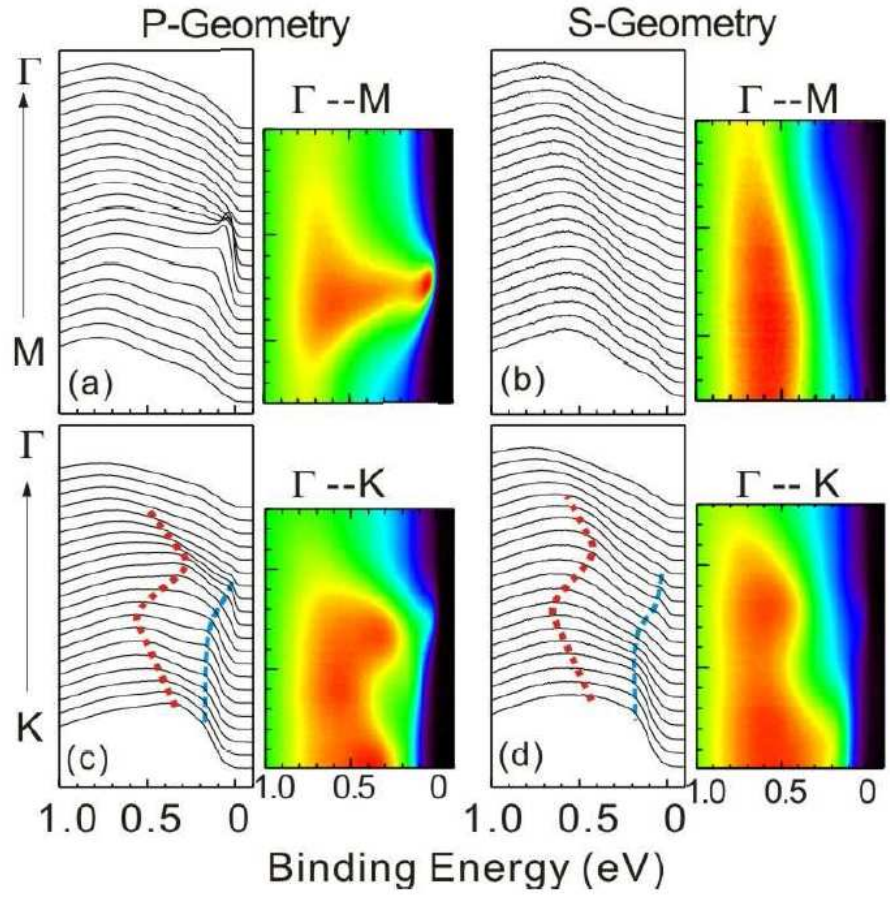




opposite charge transfer: importance of density of states!

$Na_{0.3}CoO_2$ quasi-particle bands vs ARPES



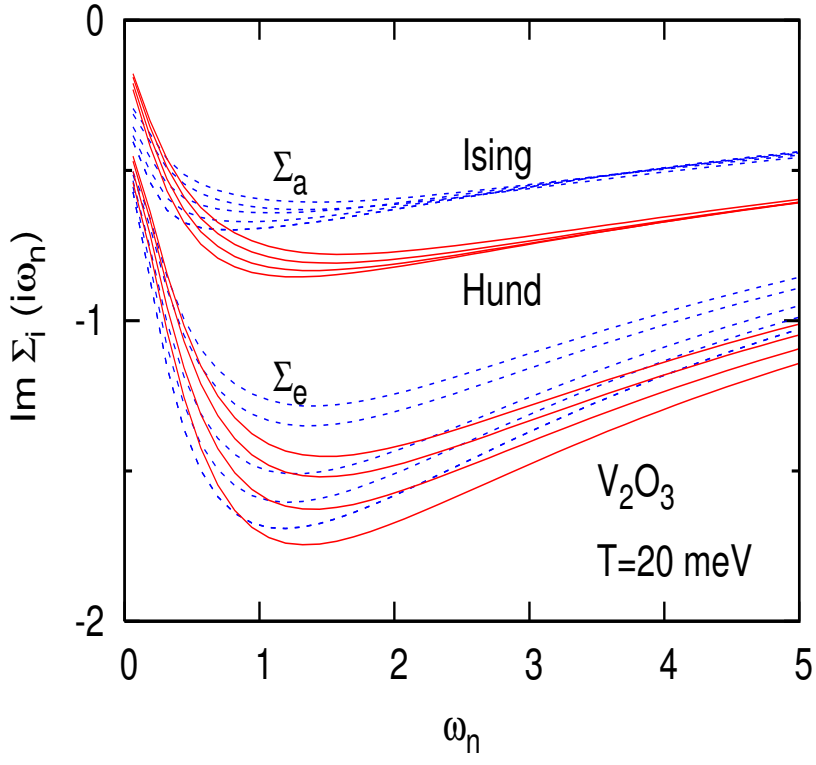


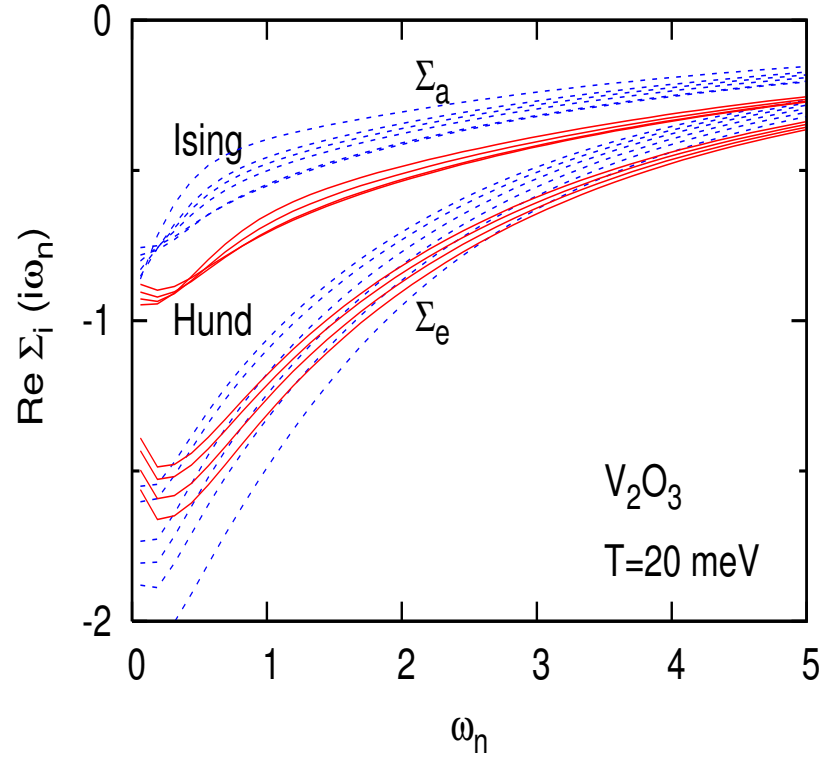
Perroni, Ishida + A.L. PRB (2007)

Qian et al PRL (2006)

~ 30 % band narrowing: $1.5 \rightarrow 1.0$ eV

V_2O_3 ED: Hund vs Ising exchange





A.L. (2007)

Ising: nearly localized e_g:
modifies (i) a_g self-energy (ii) intra-e_g scattering
(see: two-band model !)