A Fermi resonance at the $LaMnO_3$-$SrMnO_3$ interface observed with resonant soft x-ray scattering

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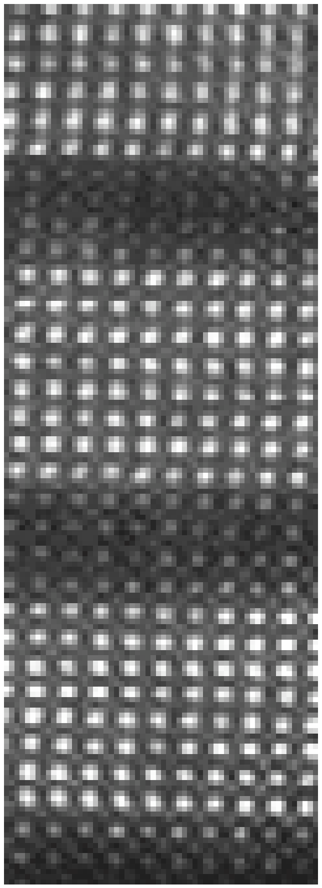

Scattering:

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Andrivo Rusydi, *University of Hamburg*
James Lee, *University of Illinois*
Shuai Wang, *University of Illinois*
Bin Jiang, *University of Illinois*
Jim Zuo, *University of Illinois*

Synthesis:

Anand Bhattacharia, *Argonne National Laboratory*
Xiaofang Zhai, *University of Illinois*
Jim Eckstein, *University of Illinois*
Genna Logvenov, *Brookhaven National Laboratory*
Ivan Bozovic, *Brookhaven National Laboratory*

S. Smadici, et al., *Phys. Rev. Lett.*, **102**, 107004 (2009)
S. Smadici, et al., *Phys. Rev. Lett.*, **99**, 196404 (2007)
P. Abbamonte, et al., Science, **297**, 581 (2002)

MRL
THE FREDERICK SEITZ MATERIALS RESEARCH LABORATORY

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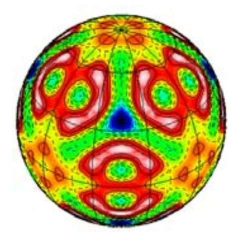
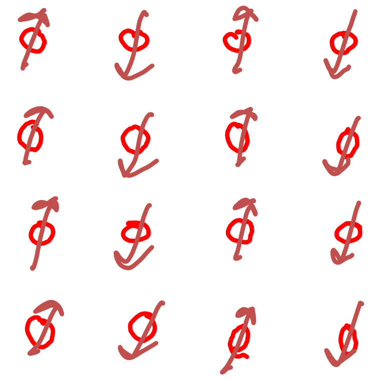
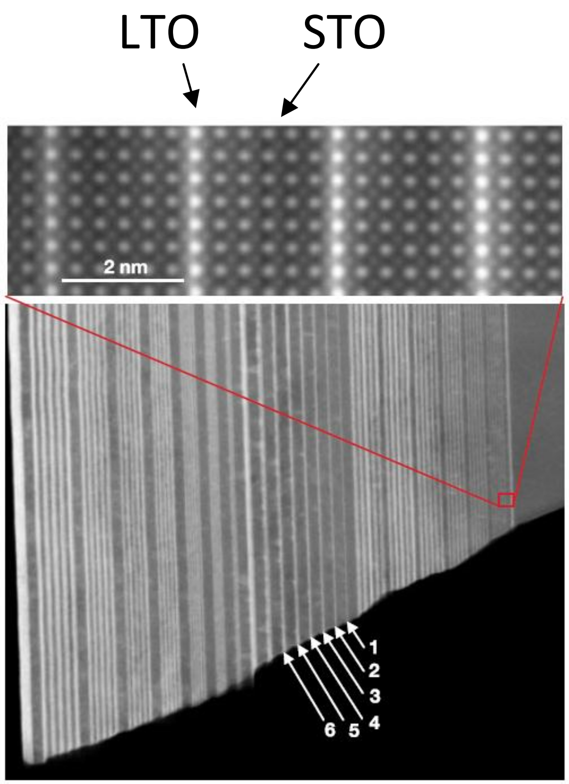


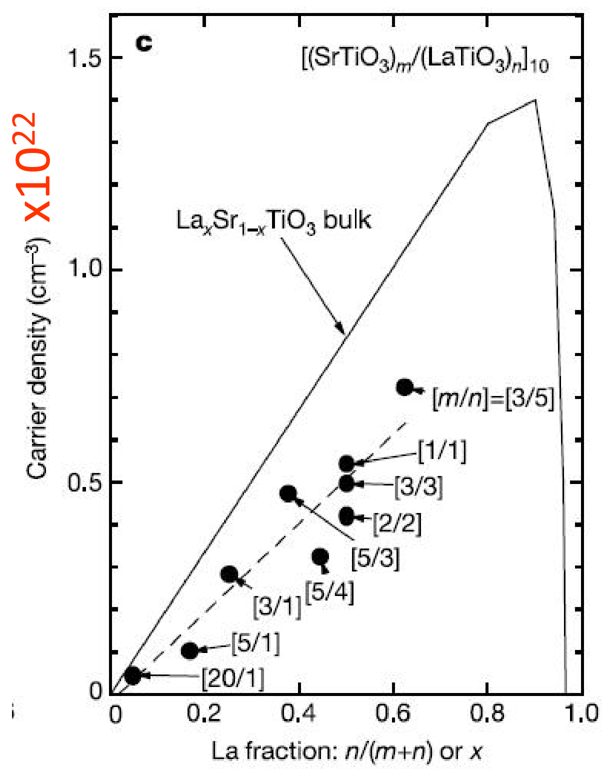
$LaTiO_3$ – $SrTiO_3$ Interface

$SrTiO_3$
d^0 band insulator

$LaTiO_3$
d^1 Mott insulator

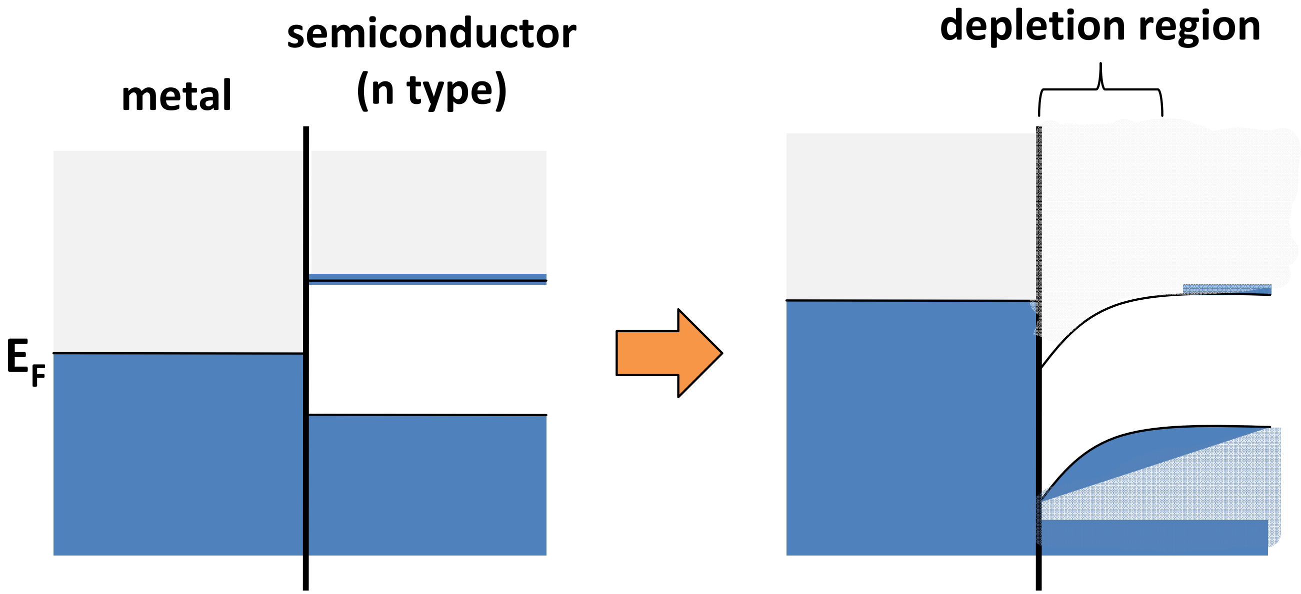




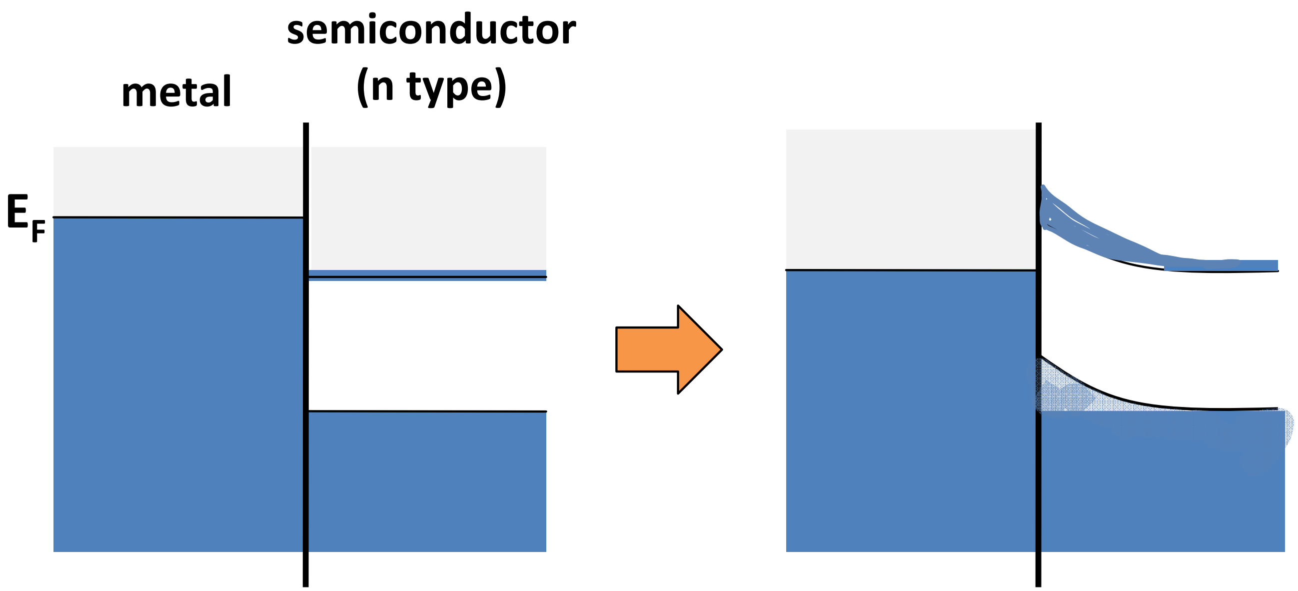


A. Ohtomo, D. Muller, J. Grazul, H. Hwang, *Nature*, **419**, 378 (2002)

Effect #1: Band lineup

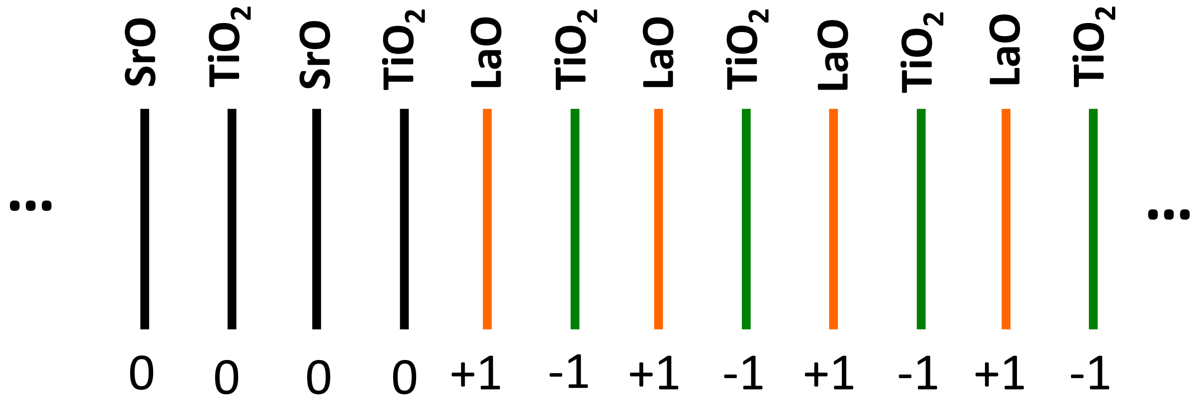


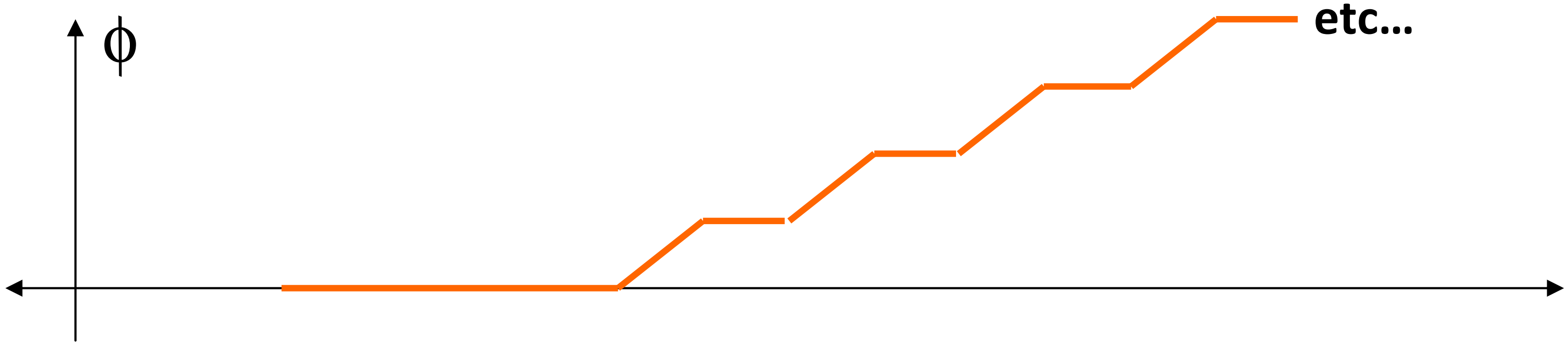
- Carrier depletion in semiconductor
- Schottky barrier
- Rectifying



- Carrier accumulation
- Ohmic contact

Effect #2: Polar Fields

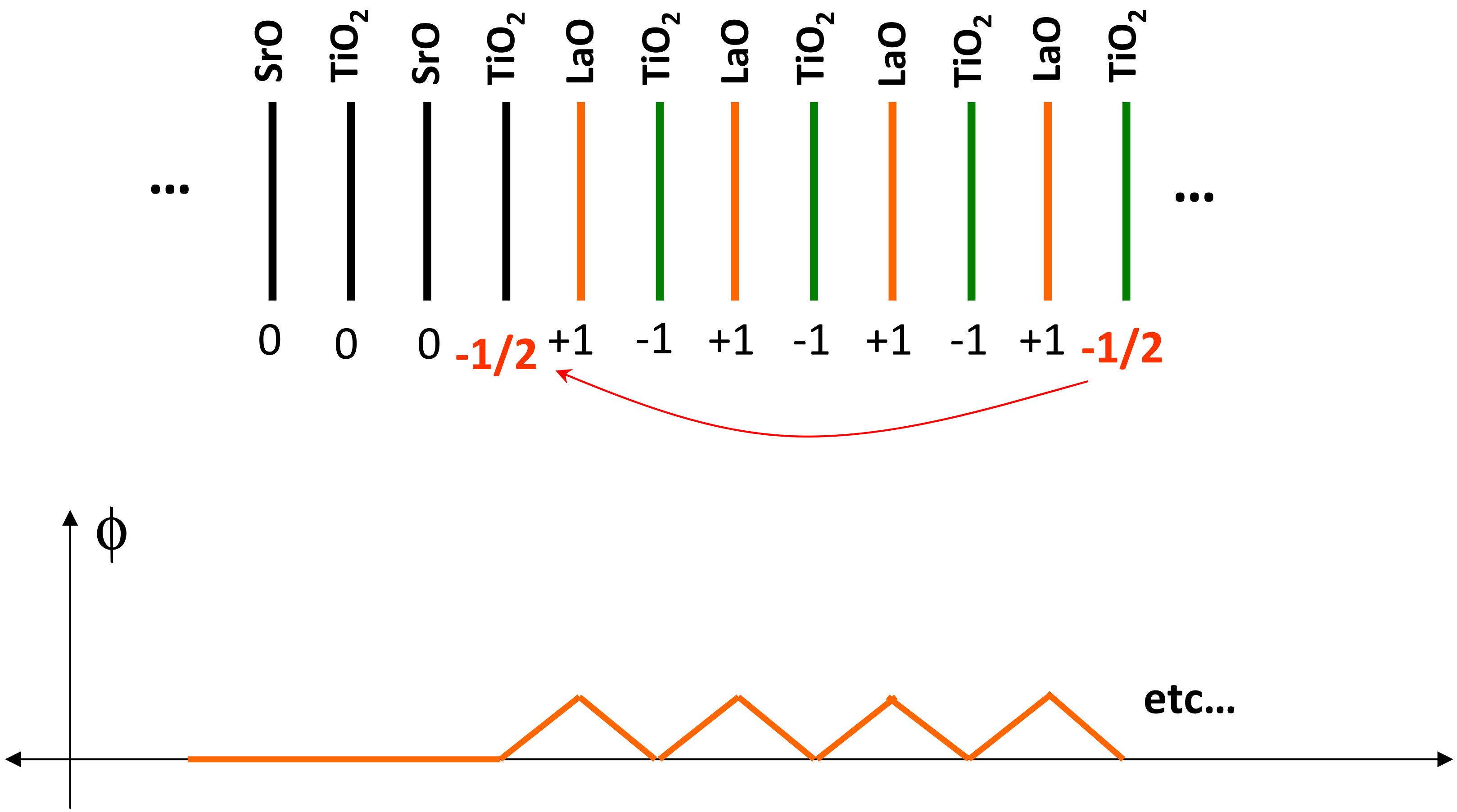




Electrostatic energy diverges; interface must

W. A. Harrison, E. A. Kraut, J. R. Waldrop, R. W. Grant, Phys. Rev. B, **18**, 4402 (1978)
R. Hesper, L. H. Tjeng, A. Heeres, G. A. Sawatzky, Phys. Rev. B, **62**, 16046 (2000)
N. Nakagawa, H. Y. Hwang, D. A. Muller, Nat. Mat., **5**, 204 (2006)

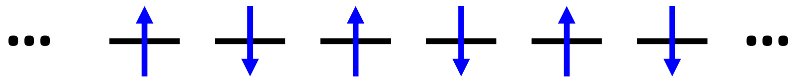
Effect #2: Polar Fields



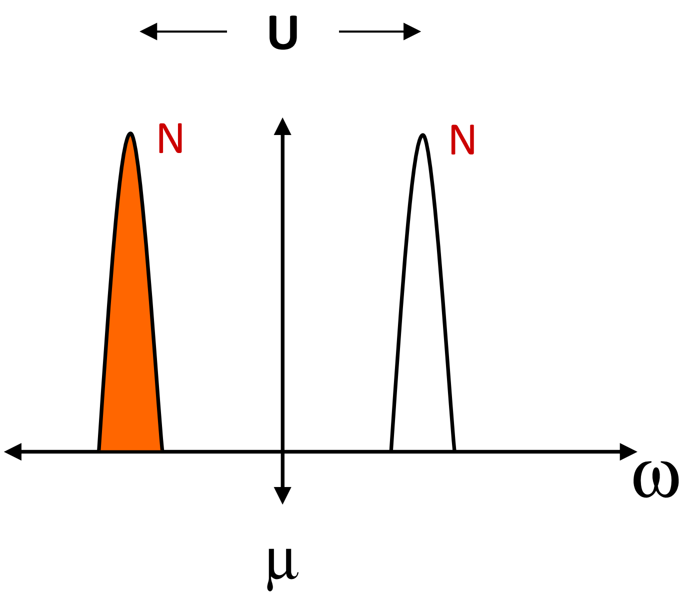
Electronic reconstruction

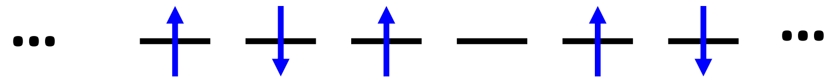
W. A. Harrison, E. A. Kraut, J. R. Waldrop, R. W. Grant, Phys. Rev. B, **18**, 4402 (1978)
R. Hesper, L. H. Tjeng, A. Heeres, G. A. Sawatzky, Phys. Rev. B, **62**, 16046 (2000)
N. Nakagawa, H. Y. Hwang, D. A. Muller, Nat. Mat., **5**, 204 (2006)

Effect #3: Spectral Weight Transfer

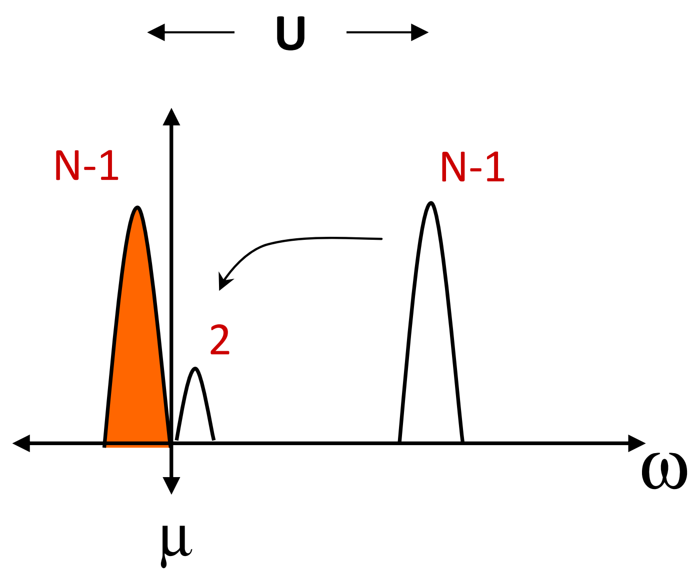


Density of states
(i.e., spectral function)



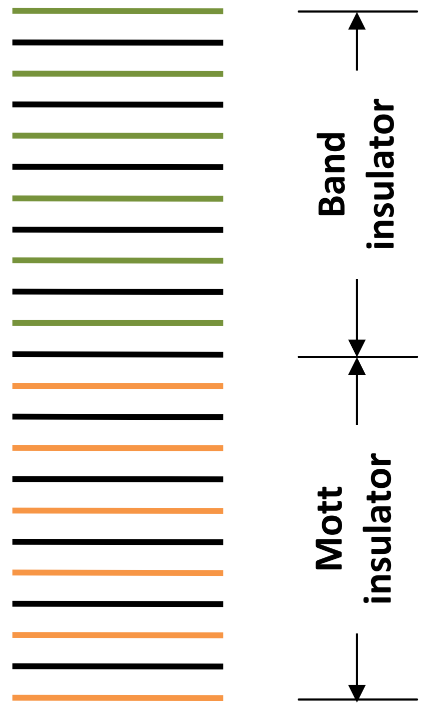


Density of states
(i.e., spectral function)

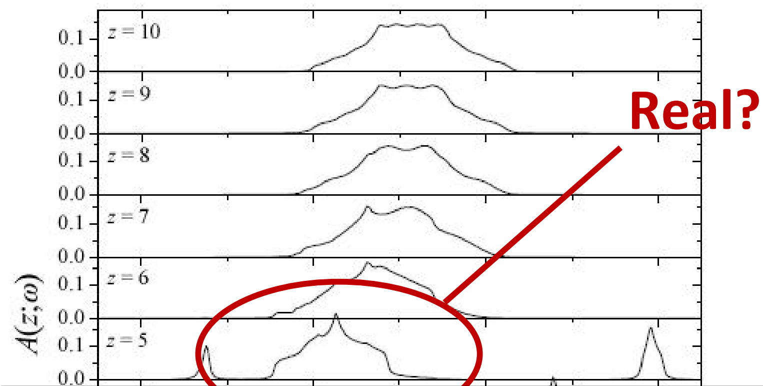


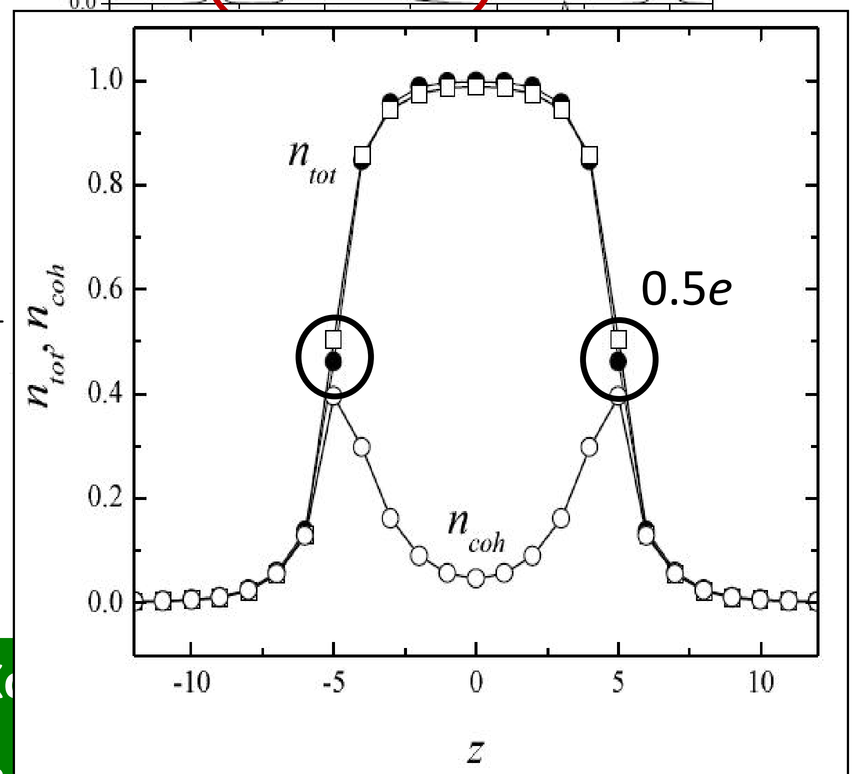
H. Eskes, M. B. J. Meinders, G. A. Sawatzky, *Phys. Rev. Lett.*, **67**, 1035 (1991)
H. Eskes, G. A. Sawatzky, *Phys. Rev. B*, **43**, 119 (1991)

$LaTiO_3$-$SrTiO_3$: Okamoto & Millis



- S. Okamoto, A. J. Millis, *Nature*, **428**, 630 (2004)
- S. Okamoto, A. J. Millis, *Phys. Rev. B*, **70**, 241104(R) (2004)
- Etc.





- $\Sigma_\sigma(\omega) = \Sigma_\sigma^H(\omega) + \Sigma_\sigma^D(\omega)$ (Hartree term
- Solve dynamical part with DMFT

Everything in DMFT is a K

Is there really a

Resonant soft x-ray scattering (RSXS)

One-electron Green's function: $G^R(i,i',t-t') = \langle 0 | [d_i(t), d_{i'}^{\dagger}(t')] | 0 \rangle \theta(t-t')$

$I_{STM}(i,\omega) = -\mathrm{Im}\left[G^R(i,i,\omega)\right]$ where $G^R(i,i,\omega)$ = time transform of $G^R(i,i,t-t')$

$I_{ARPES}(k,\omega) = -\mathrm{Im}\left[G^R(k,\omega)\right]$ where $G^R(k,\omega)$ = space-time transform of $G^R(i-i',t-t')$

What about RSXS? … Assumptions:

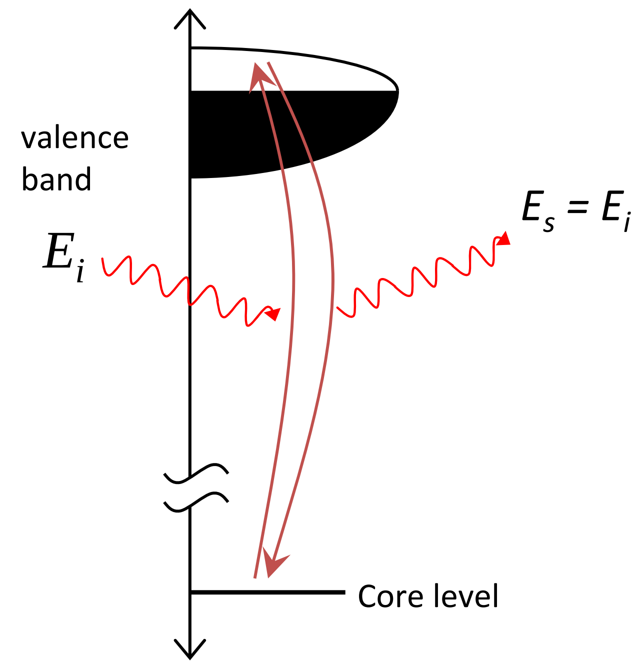
- Only elastic processes
- Core hole does not propagate (local scattering only)
- Neglect excitonic effects

$$\rho_{\mathbf{q}} = \frac{1}{V_{cell}} \sum_n f_n e^{i\,\mathbf{q}\cdot\mathbf{r}_n}$$

$$\hat{V} = \sum_i d_i^{\dagger} c_i a_k e^{i\mathbf{k}\cdot\mathbf{r}_i} + h.c.$$

$$I_{RSXS}(\mathbf{q},\omega) = \left| \sum_{i,n} \frac{<0|d_i|n><n|d_i^{\dagger}|0>}{\omega + \varepsilon_{core} - \varepsilon_n^{N+1} + i\eta} e^{-i\mathbf{q}\cdot\mathbf{r}_i} \right|^2$$

$$G^R(i,i,\omega) = \sum_{i,n} \frac{<0|d_i|n><n|d_i^{\dagger}|0>}{\omega - \varepsilon_n^{N+1} + i\eta} + \frac{<0|d_i^{\dagger}|n><n|d_i|0>}{\omega + \varepsilon_n^{N-1} + i\eta}$$



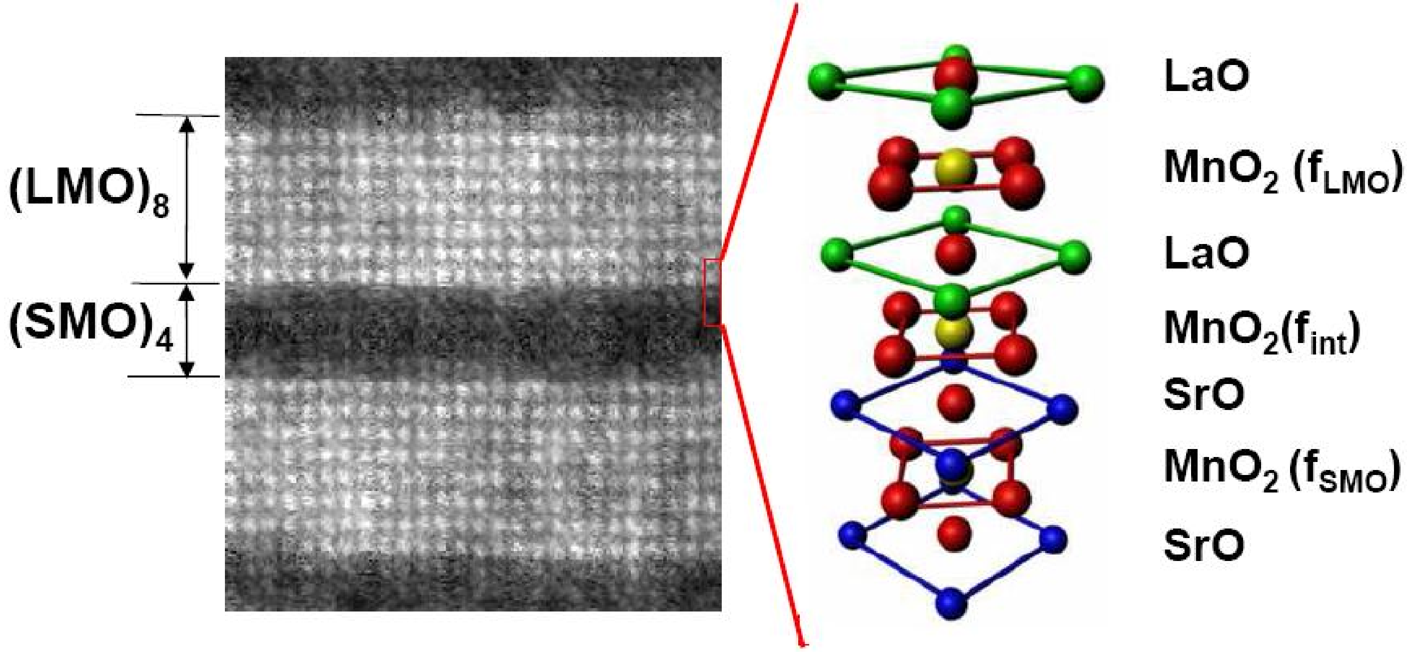
$$I_{RSXS}(\mathbf{q},\omega) = \left| G^R(\mathbf{q}, \omega - \omega_{core}) \right|^2$$

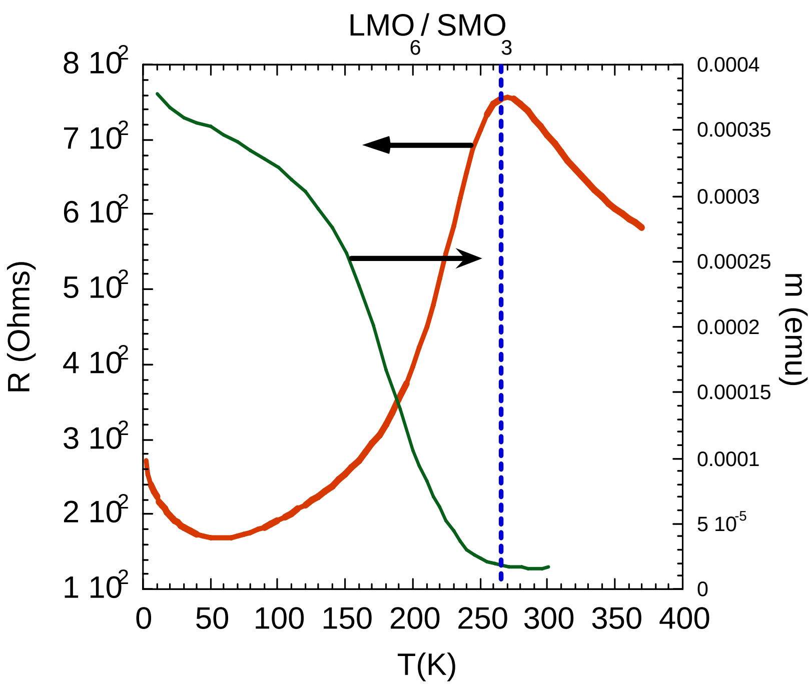
(Thanks to Eugene Demler for the quantitative argument)

$LaMnO_3 – SrMnO_3$

$LaMnO_3$
$t_{2g}^3 e_g^1$
Mott insulator

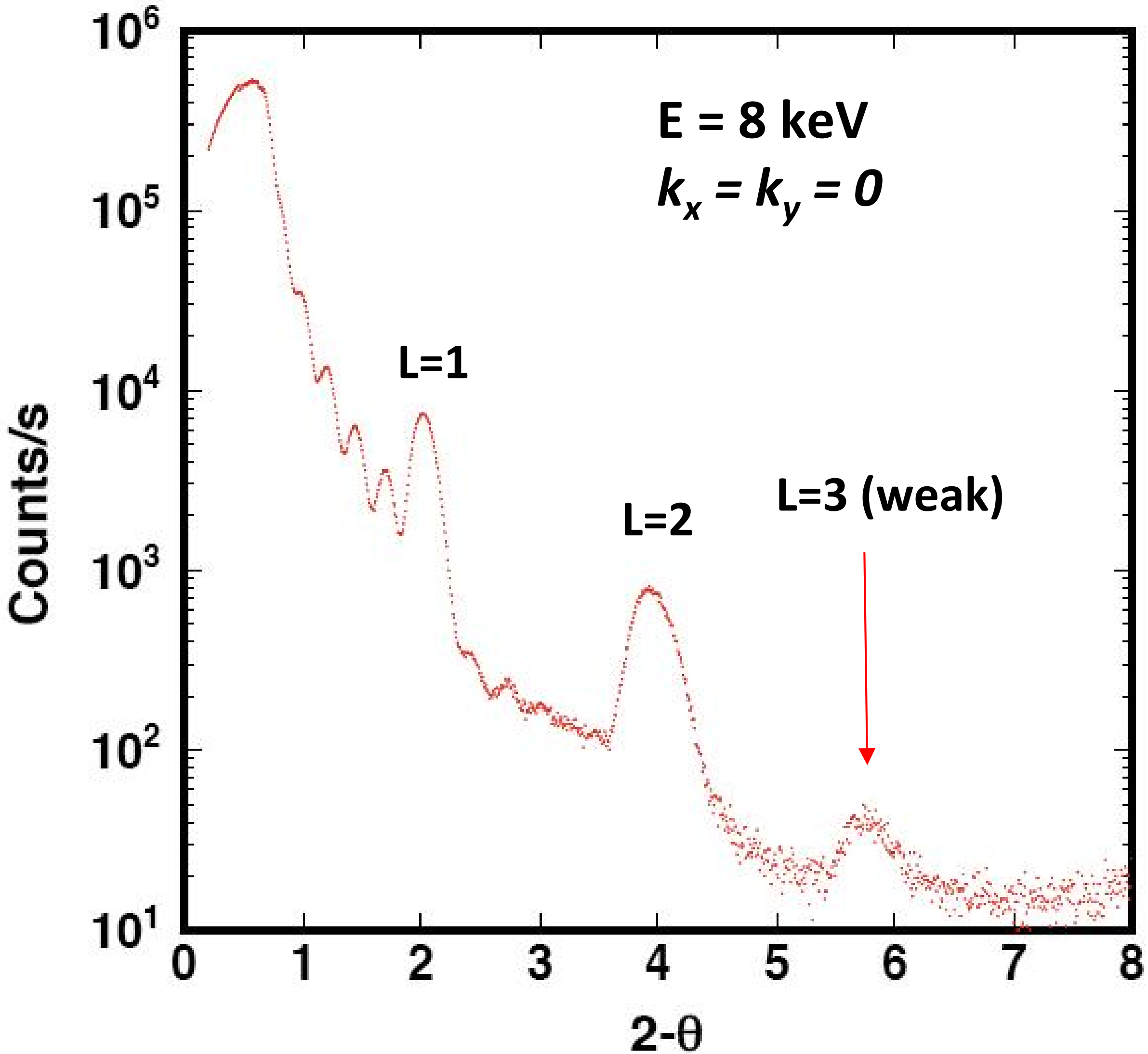
$SrMnO_3$
$t_{2g}^3 e_g^0$
"Band" insulator





- MBE
- Metallic (like $LaTiO_3$-$SrTiO_3$)
- Ferromagnetic!
- Double-exchange FM at interfaces.
- *Okamoto-Millis peak?*

Extinction rules



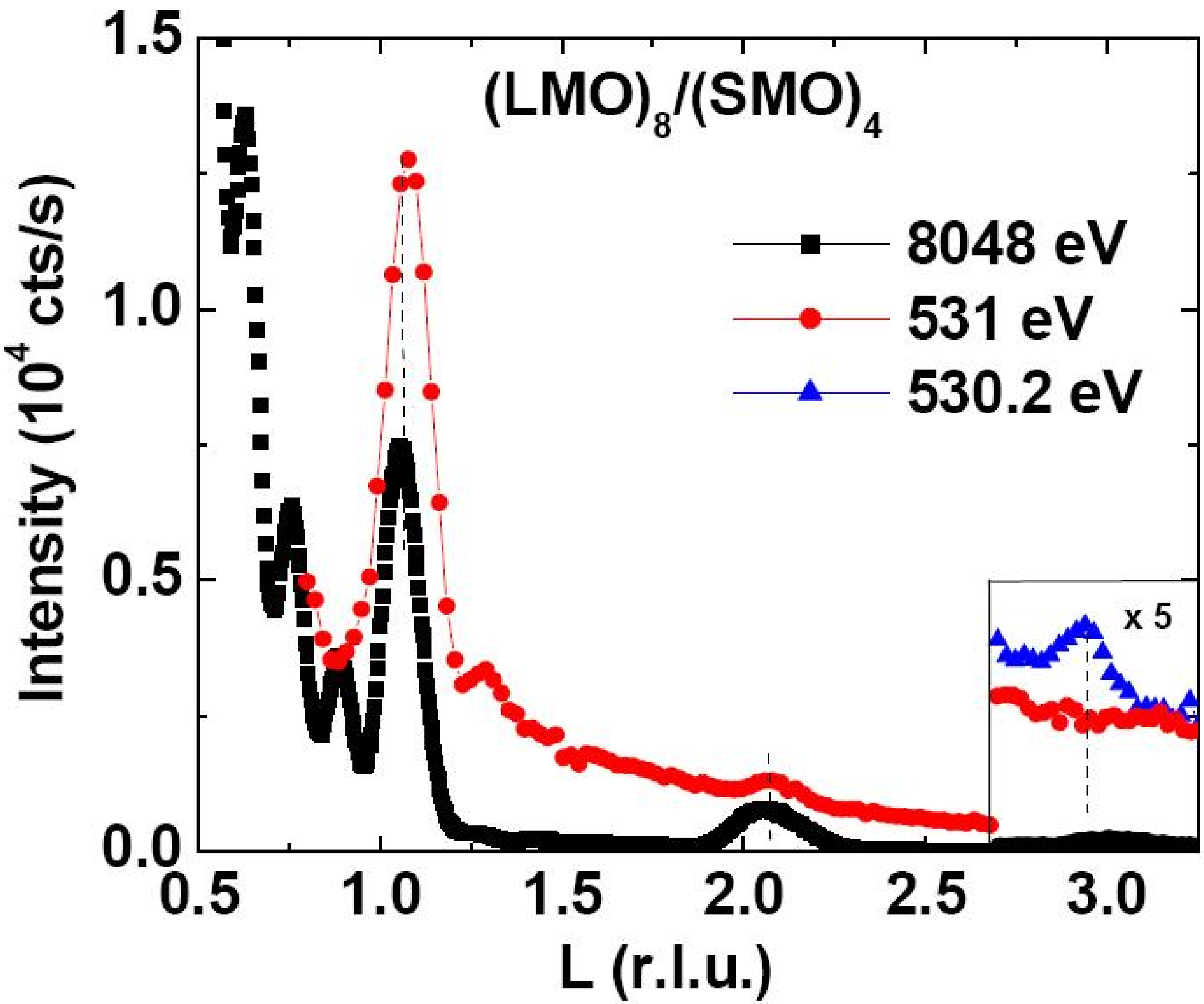
$$\rho_{\mathbf{q}} = \frac{1}{V_{cell}} \sum_n f_n e^{i\,\mathbf{q}\cdot\mathbf{r}_n}$$

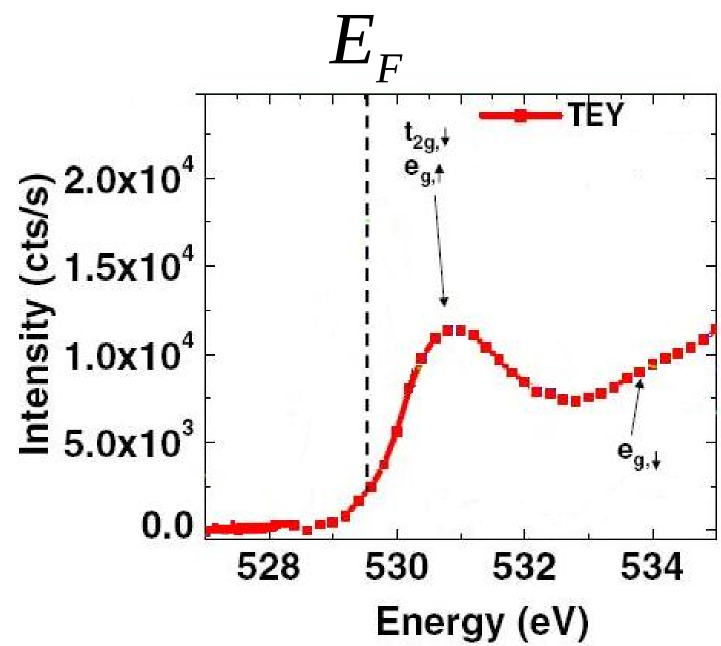
$$G = 2\pi\left(H/a, K/b, L/c\right)$$

$$\rho_3 = 2\,f_{\text{int}} - f_{LMO} - f_{SMO}$$

- 6% of sample defect phases (7/4, 8/5, etc.)
- Directly sensitive to interface density of states

RSXS results

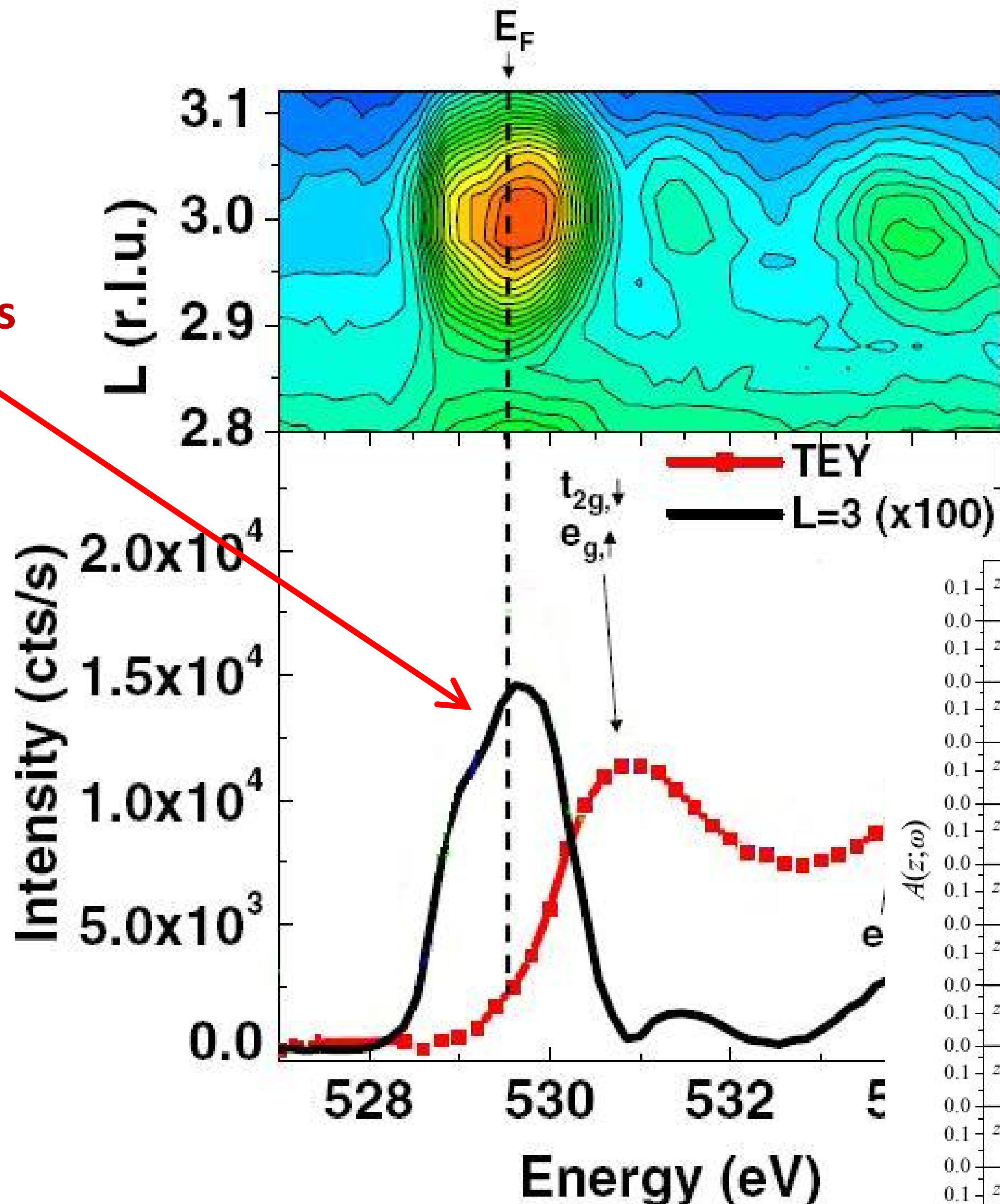




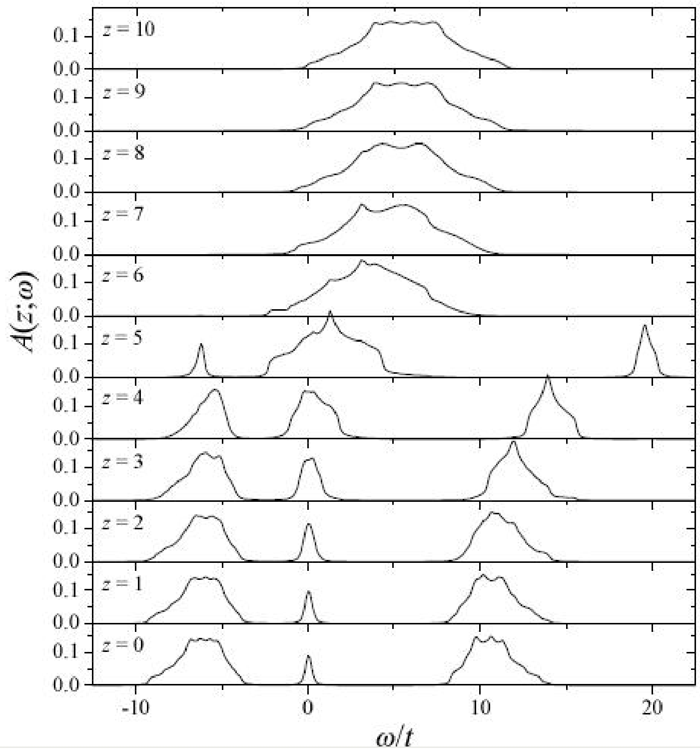
$$\mathbf{q} = 2\pi\left(0,0,L/c\right)$$

Results

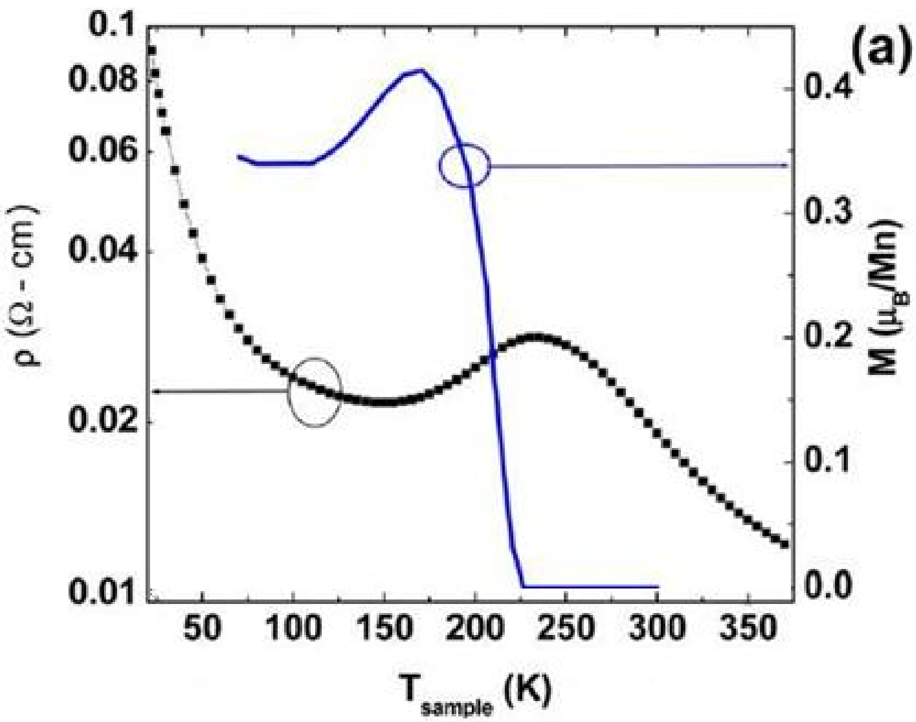
Okamoto-Millis
Peak
(?)

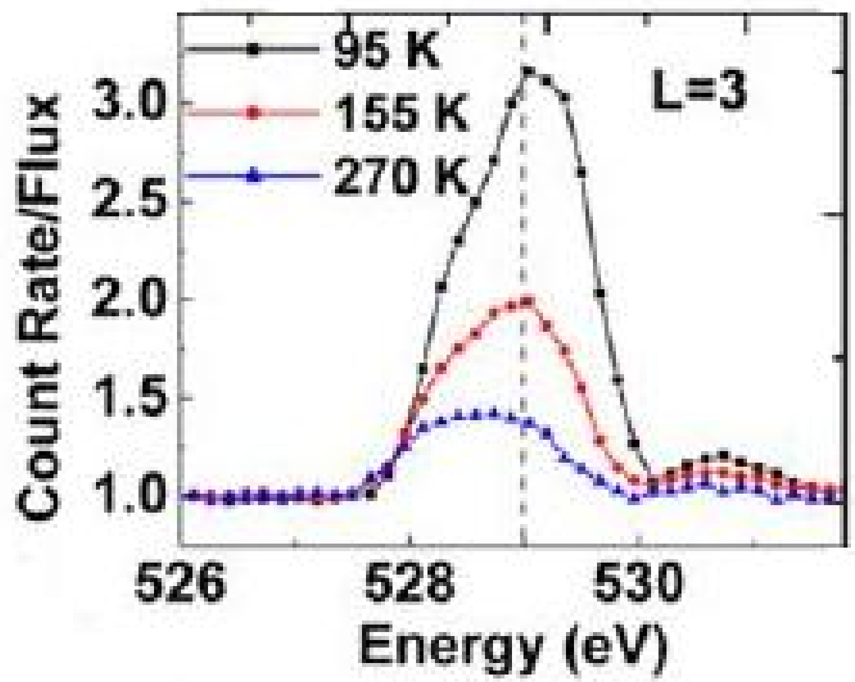


S. Smadici, PRL 99



Temperature dependence

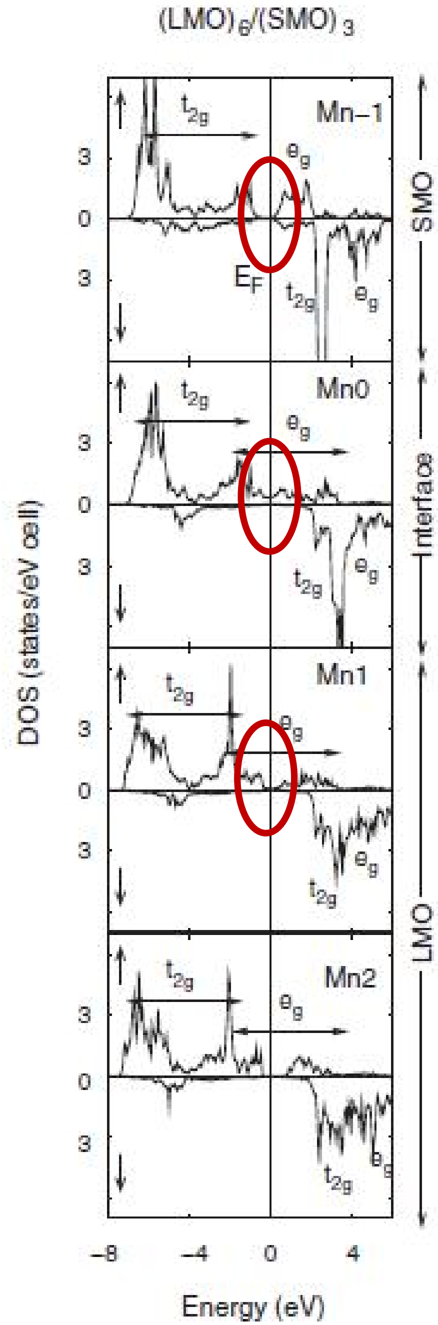




Feedback between Fermi resonance and interface mobility

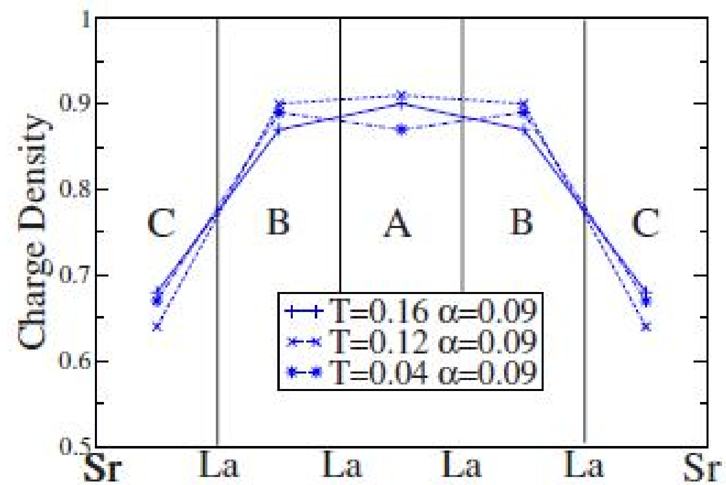
S. Smadici, PRL, **99**, 196404 (2007)

Possible theoretical "postdiction"



GGA+U

B. R. K. Nanda, S. Satpathy, PRB, **79**, 054228 (2009)



(orbital ordering but not magnetic ordering presented), and 0.04t (both orbital and magnetic orders). The variation in charge distribution for different temperatures is smaller than 5%. We note that very recent x-ray scattering experiments on manganite superlattice[28] indicate a large change in L and K edge absorption intensities as the temperature is decreased through the Curie temperature. If the experiments measure the total interface charge density, they may be in contradiction to our results, but if data are proportional to the near-Fermi-surface coherent excitations (which grow below Curie temperature according to our calculation), there may not be a contradiction.[29]

The staggered Q_x order. Table I lists the layer charge density, the computed SL Q_x order, and the bulk Q_x order at the given layer charge density of the (4,1) SL for α=0.3 and

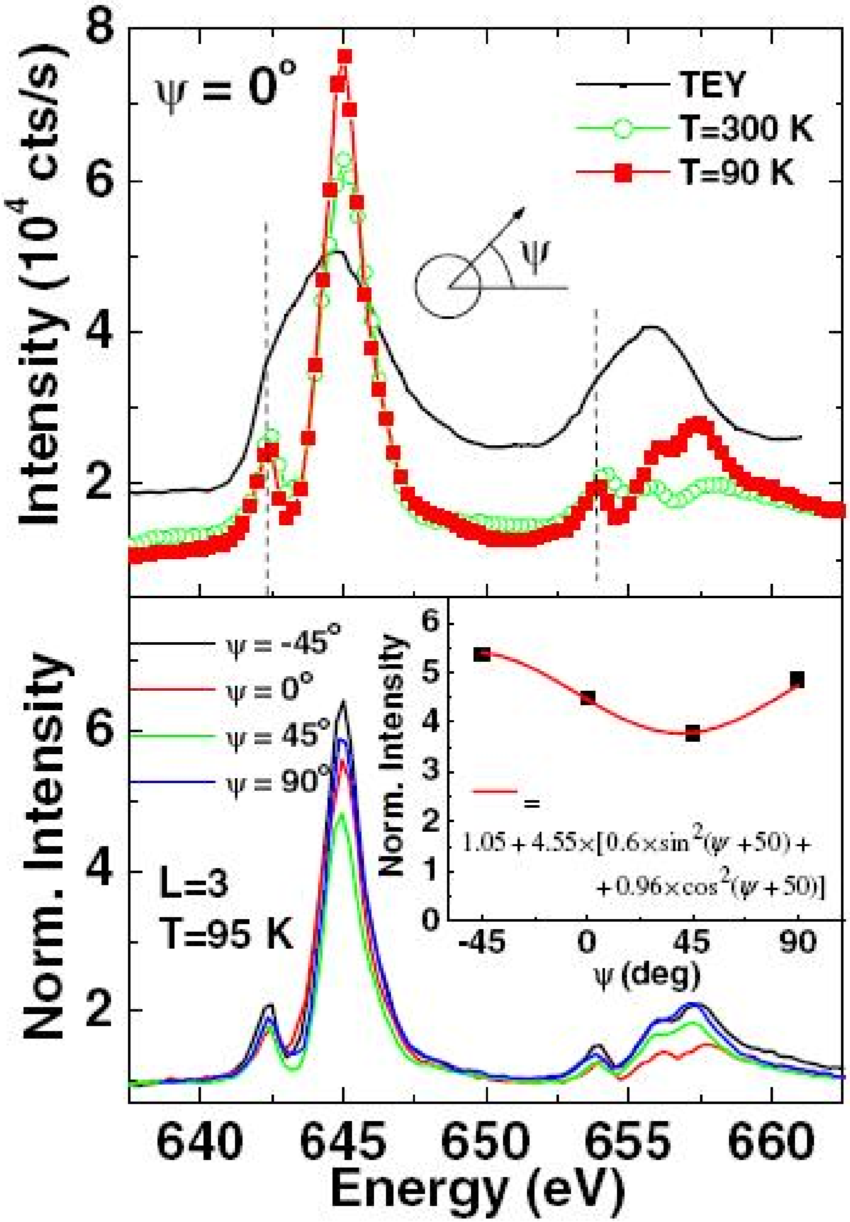
DMFT + Poisson eq.

C. Lin, A. J. Millis, PRB, **78**, 184405 (2008)

Conclusions

- $LaMnO_3$ and $SrMnO_3$ are insulators, but their interface is metallic. (like LTO-STO)
- Metallic behavior occurs through transfer of spectral weight from high energy
- Ferromagnetic too - interface double-exchange.
- Evidence for Okamoto-Millis-like peak. Theoretical “postdiction” looks promising.

Magnetic scattering @ $MnL_{3/2}$ edge



$$M \sim \mathbf{S} \cdot (\hat{\varepsilon}_f^* \times \hat{\varepsilon}_i)$$

$$I \propto \cos^2(\theta)\sin^2(\psi) + \sin^2(2\theta)\cos^2(\psi)$$

- Magnetic scattering resembles mod squared of XMCD
- Moment 50° from Mn-O bonds
- Detailed line shape difficult to disentangle