?What are the physics questions?

- **charge transfer:**
  - **--how much charge moves?**
  - **-- how far?**
  - **--into what orbitals?**
  - **--causing what lattice relaxations?**
- **order parameter transfer:**
  - **--penetration depth**
  - **--domain walls between different kinds of order**
- **"new" phenomena:**
  - **--interface spin/charge/orbital/sc order**
  - **--Parkin question: room temp SC?**
- **dynamics:**
  - **--linear + nonlinear response**
  - **--control=>?devices**

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Theoretical Techniques

- **Basic problem: need to solve spatially inhomogeneous correlated electron system—but even homogeneous systems are notoriously difficult to treat**

1 dimension: numerics; exact solutions

D>1: mean field approximations:

***Hartree (LDA (+U))**

***Dynamical mean field**

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The (theoretical) methods

- **Band theory (and LDA +U)**
  - **--charge density**
  - **--lattice distortions**
  - **--ground state phase diagram**
- **Hartree Fock**
  - **--charge distribution**
  - **--phase diagram**
- **Many body methods (Must treat multiplet interactions)**
  - **--Spectral functions**
  - **--phase diagram**
  - **--dynamics**

Opportunity (challenge) to theory:
new system--what can be predicted?

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Density Functional Theory

Basic Theorem (Hohenberg and Kohn): $\exists$ functional Φ of electron density n(r): minimized at physical density; value at minimum gives ground state energy

$$\Phi[\{n(r)\}] = \Phi_{univ}[\{n(r)\}] + \int (dr) V_{lattice}(r) n(r)$$

Useful because:

***Have uncontrolled (but apparently good) approximations to Φ**

***Have efficient way to carry out minimization**

LDA+U: Further approximation: add Hartree interaction to LDA energy (and subtract double-counting term)

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Density functional theory: II

LDA (+U) probably not reliable for phase diagram, excitations (esp near density 1/cell)

LDA (+U) probably is reliable for charge density, basic hybridization effects (esp away from density 1/cell)

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Reasonable goal:

Use DFT to define Hamiltonian to study with many-body methods

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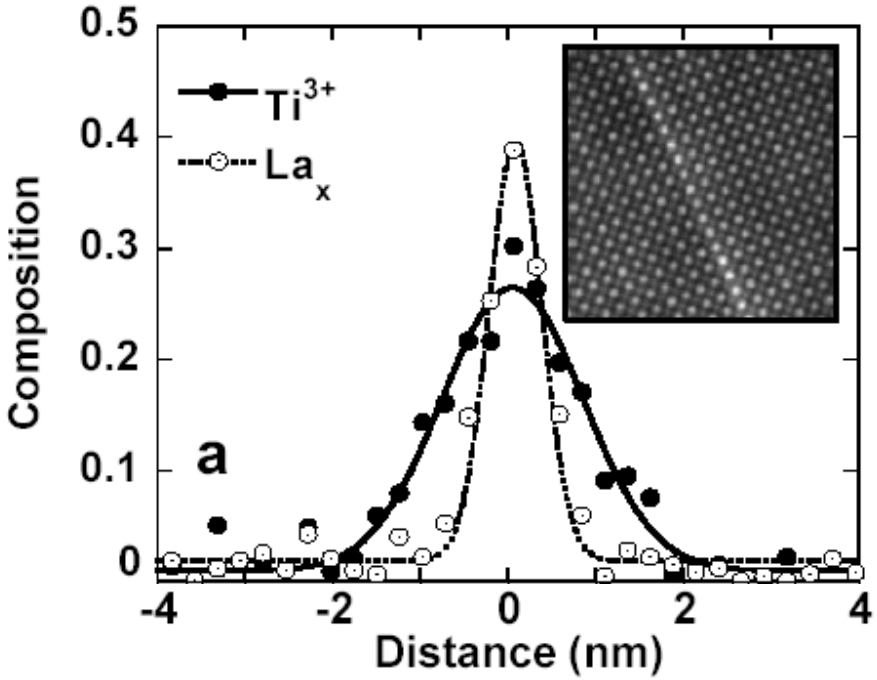
Charge Profile=>Lattice distortions



- =>dipole layer
- =>? Large coulomb forces on atoms
- =>?Structural distortions+screening

Ohtomo et al 2002

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Lattice affects density profile
density profile affects lattice

Particular issue: $SrTiO_3$ --nearly ferroelectric=>

Long distance, low T: $\epsilon > 10^3$

?But on the scale of a lattice constant?

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General issue

Proximity to interface breaks symmetry.

- **level splitting.**
- **Changes in hopping.**

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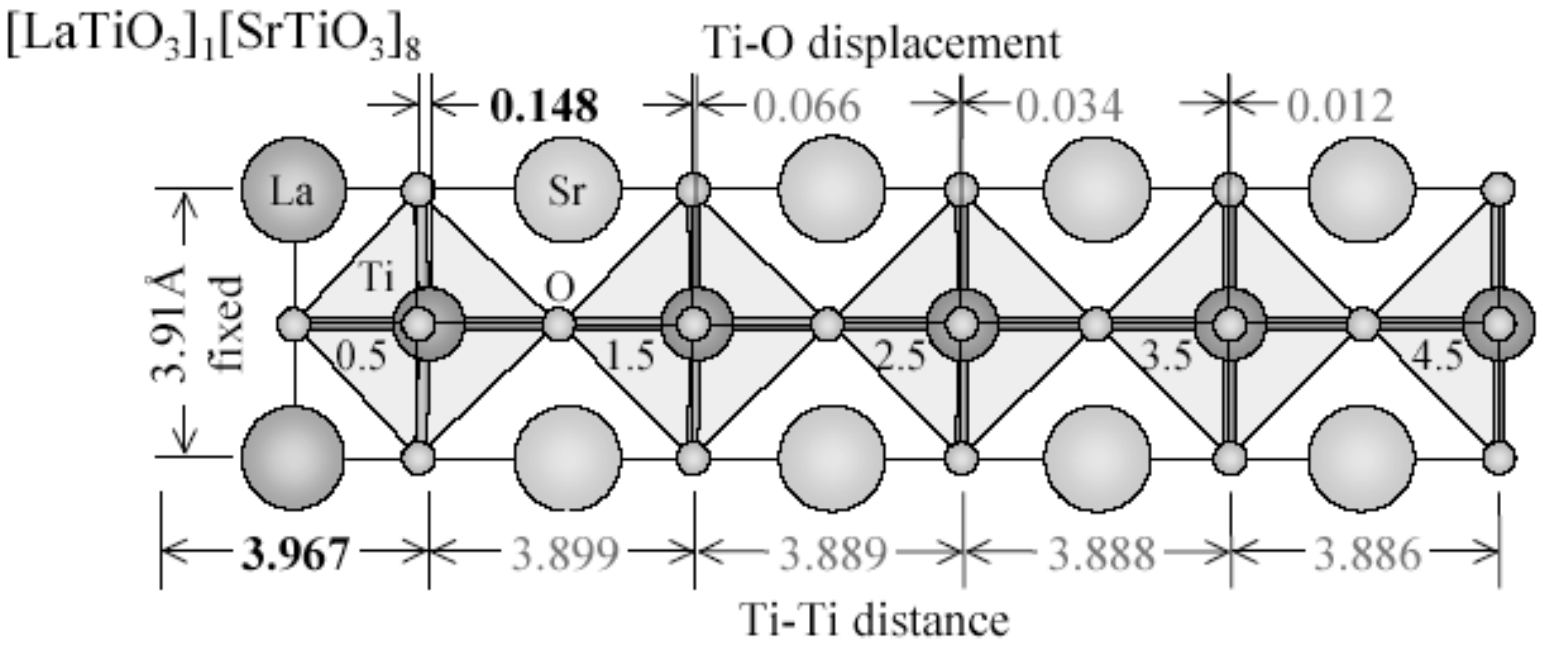
Example: 1(La)/8(Sr) Heterostructure
L(S)DA +U (VASP; U=5eV; J=0.64eV)
Relax atoms (perpendicular to plane)



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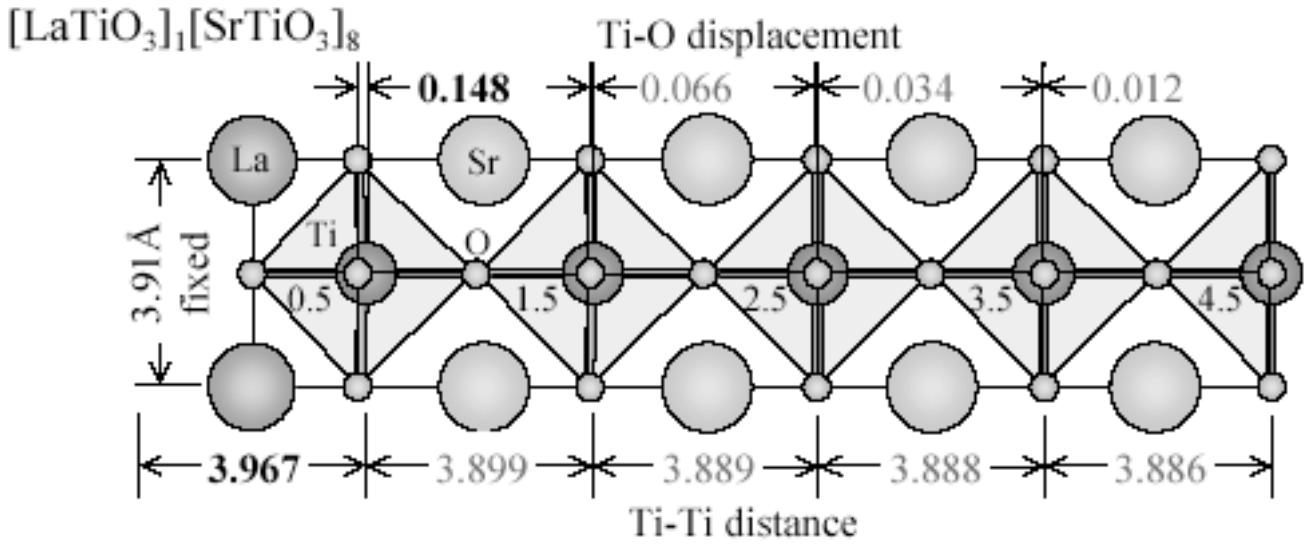
Key Results



- **Relaxation negligible in far region**
- **Near La layer: substantial distortion**
  - **"Near La" octahedra: Ferroelectric distortion**
  - **`Change in z-direction Ti-Ti bond lengths**
  - **Note in-plane O moved out of alignment**

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Electron density: how to understand results of band calculation??

- Output: atomic positions, charge density, too many bands to interpret
- charge density: includes some filled bands (those not treated as part of atomic core) =>interpretation unclear
- alternative: all electron. Draw sphere around Ti. Result depends on radius of sphere.

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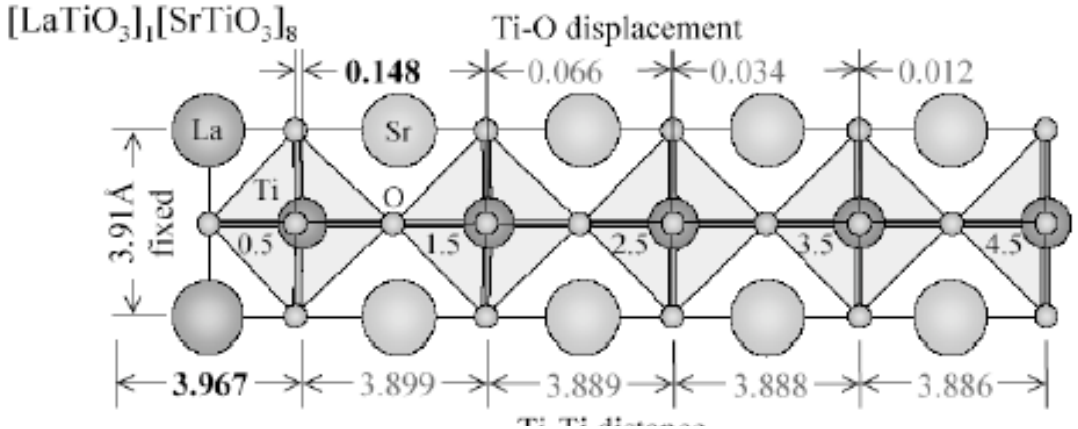
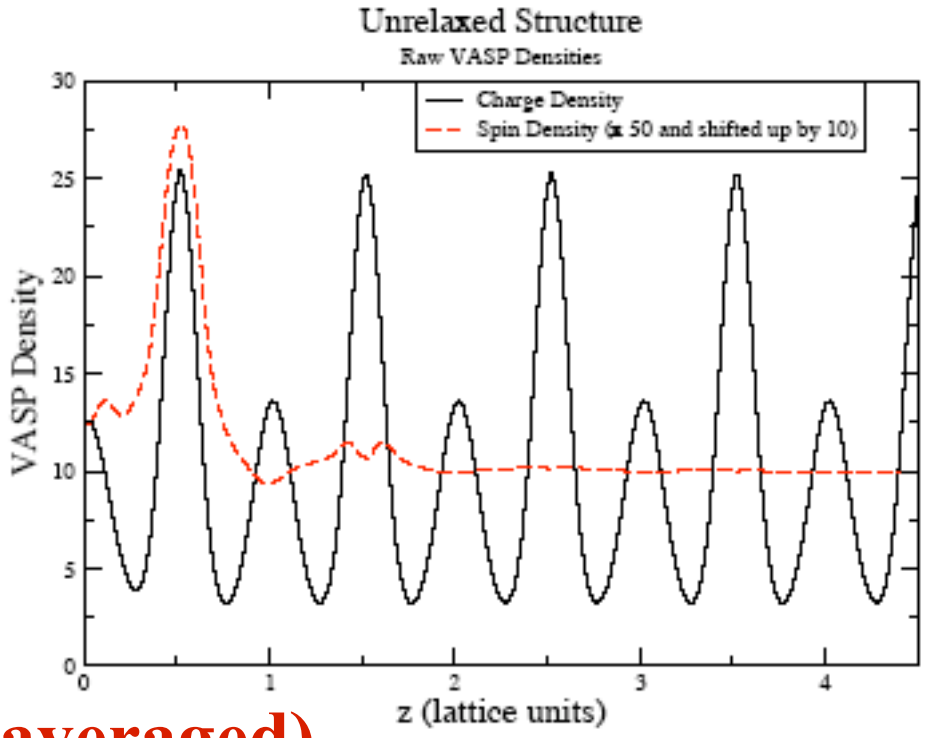
LDA+U: 1/8 heterostructure





(xy averaged)

***Charge near Ti, O**

***Spin near Ti**

***Spin decays fast**

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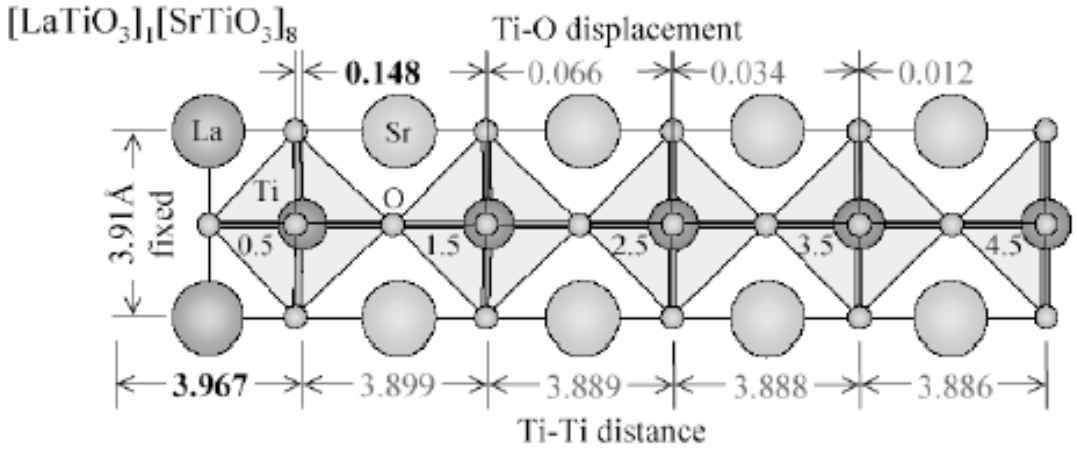
Interpret results: II



- **Spin density easy to interpret: centered on Ti.**
- **Charge density: average over unit cell (boundary=midpoint of Ti-Ti bond)**
- **Measure charge density difference from central (farthest from La) layer.**

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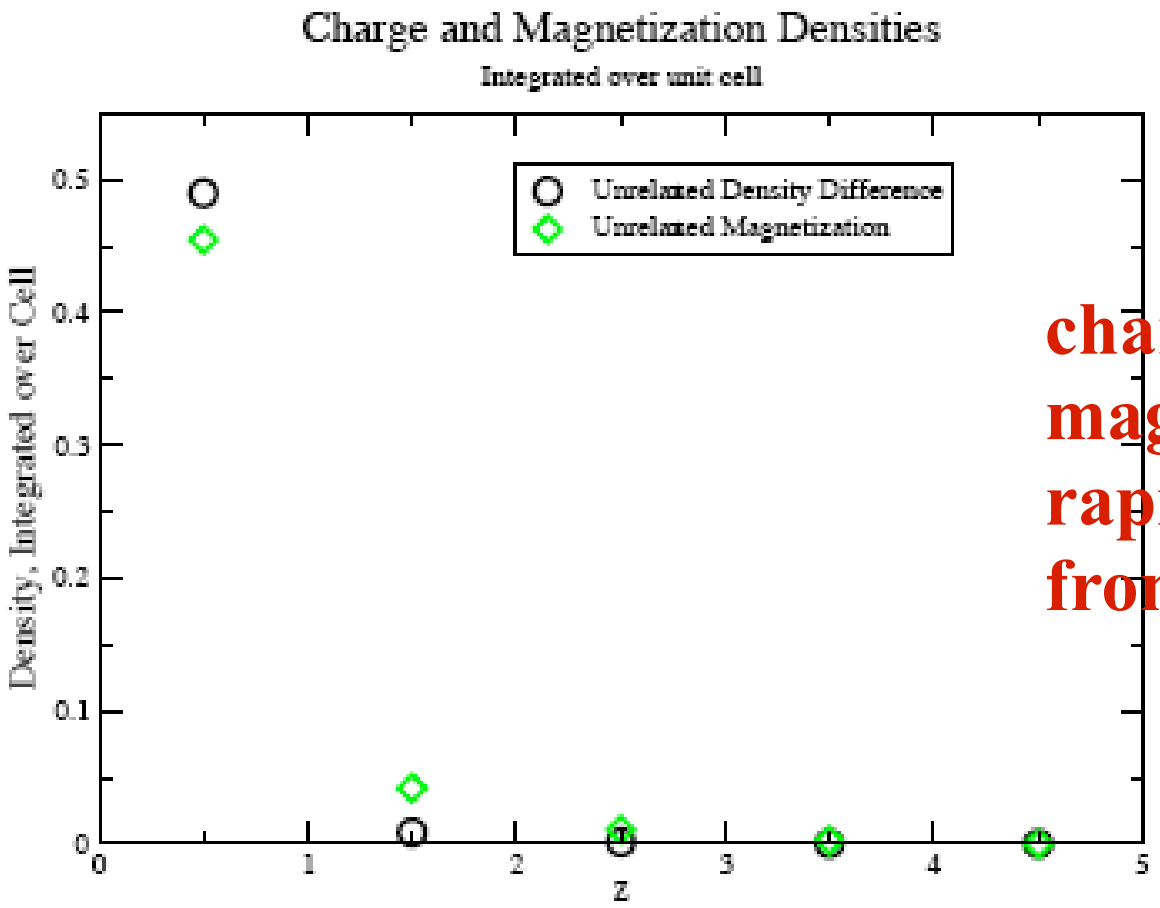
Charge and magnetization density unrelaxed heterostructure



charge and magnetization agree: rapid decay away from La layer

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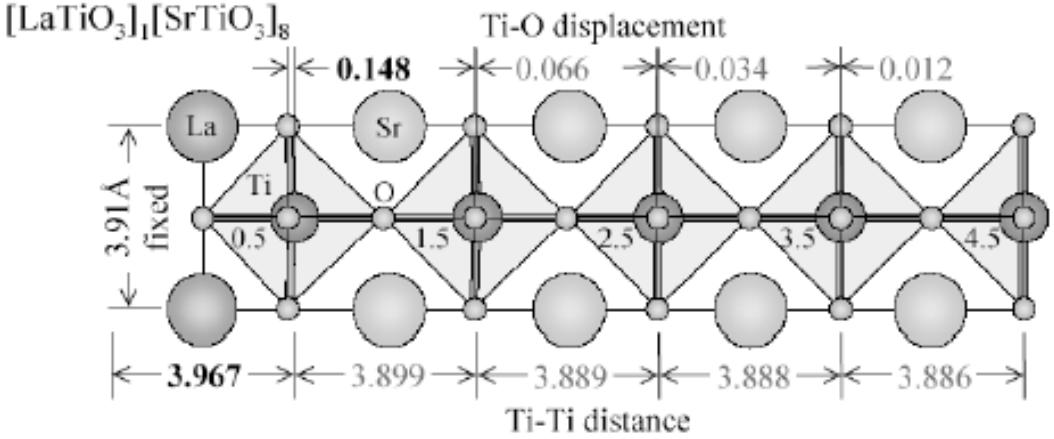
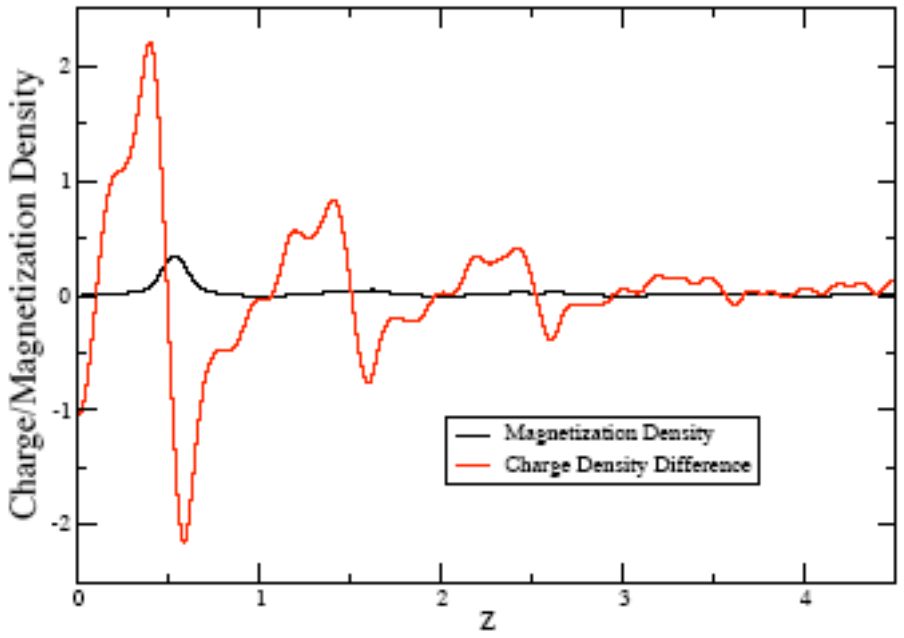
Relaxed structure:





Change in charge density extends away from La plane

Change associated with atomic motion

Question: which part comes from the "conduction" bands?

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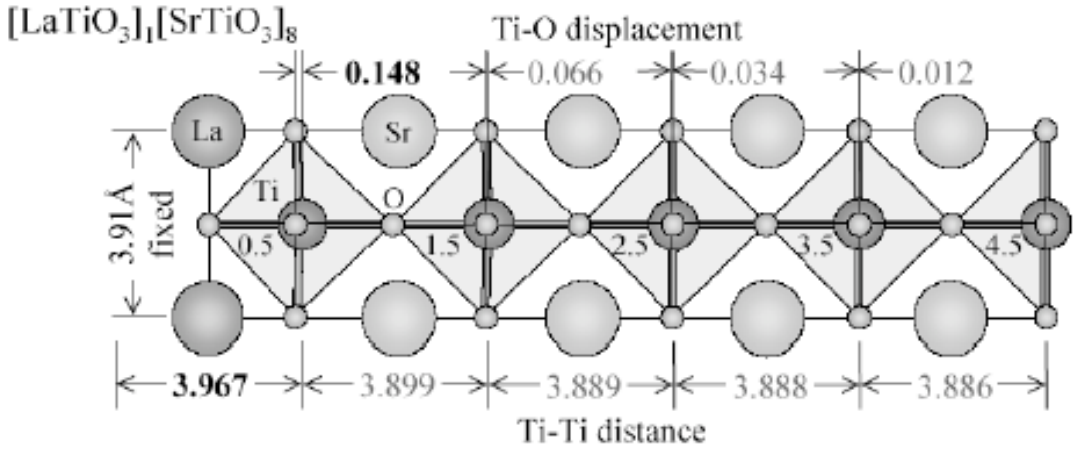
Interpret results: III



- **Spin density easy to interpret: centered on Ti.**
- **Charge density: average over unit cell (boundary=midpoint of Ti-Ti bond)**
- **Measure charge density difference from central (farthest from La) layer.**

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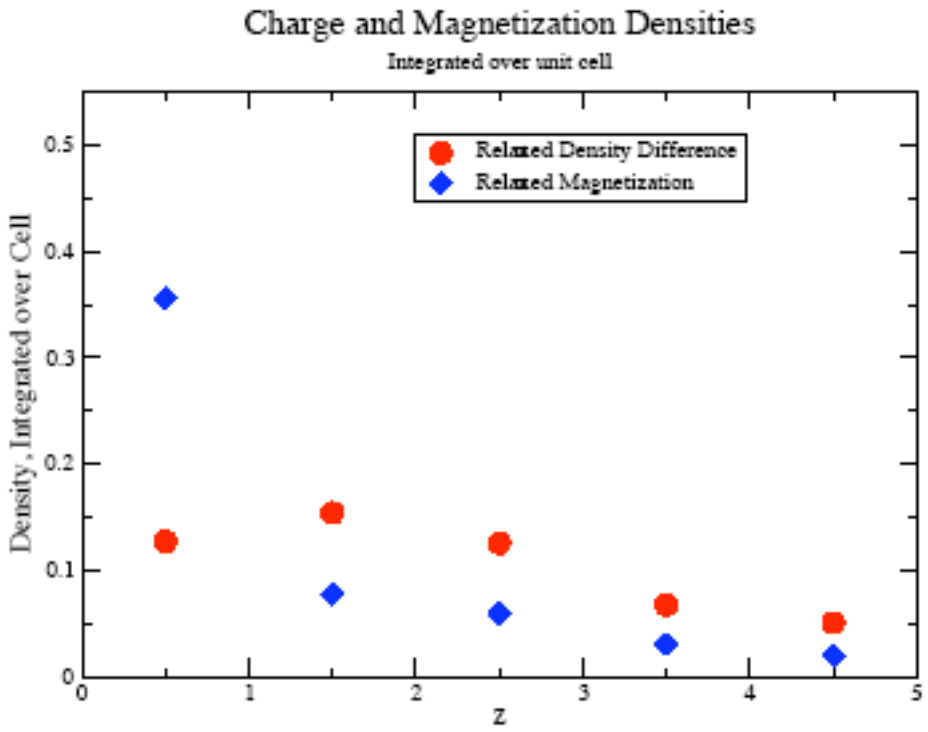
Average over unit cell



Magnetization (<=> conduction band charge): initial sharp drop; then slow decay=>scale dependent dielectric constant

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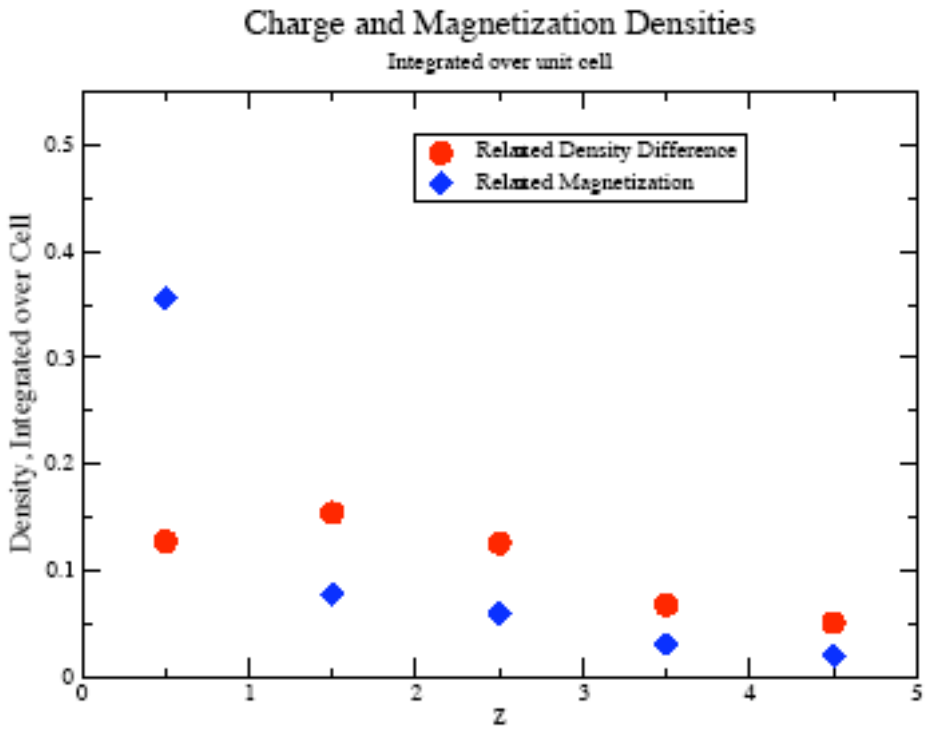
Average over unit cell



Note! charge density varies much less dramatically than magnetization. 'Bound charge' compensates for free charge.

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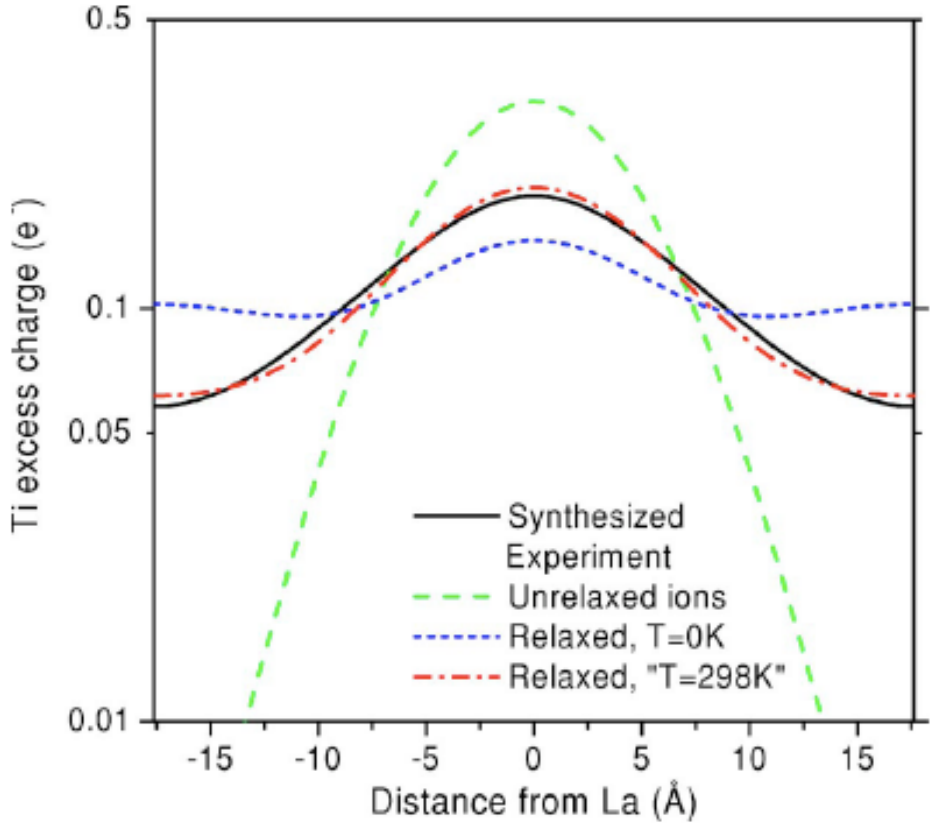
Slightly different result

PHYSICAL REVIEW B 73, 195403 (2006)

Lattice-polarization effects on electron-gas charge densities in ionic superlattices

D. R. Hamann,[1,2,3] D. A. Muller,[4] and H. Y. Hwang[5,6]



GGA + .65A sphere around Ti

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Compare to model system calculations

tight binding + self consistent potential

$$-\sum_{ijab\sigma} t_{ij}^{ab} d_{i,a,\sigma}^{\dagger} d_{j,b,\sigma}$$

$$V(R_i) = -\sum_{j} \frac{e^2}{\epsilon \left| \vec{R}_i - \vec{R}_j^A \right|} + \sum_{j\sigma} \frac{e^2 \left\langle n_{j\sigma} \right\rangle}{\epsilon \left| \vec{R}_i - \vec{R}_j \right|}$$

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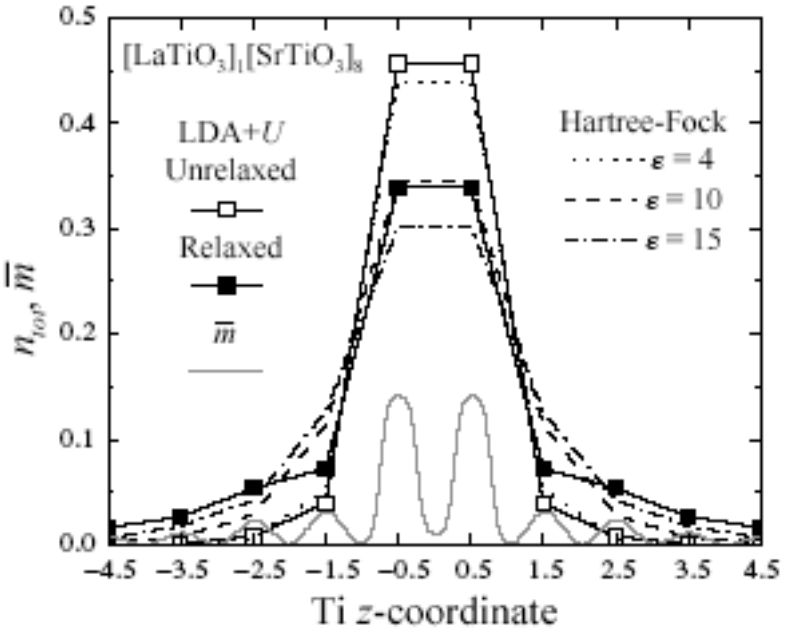
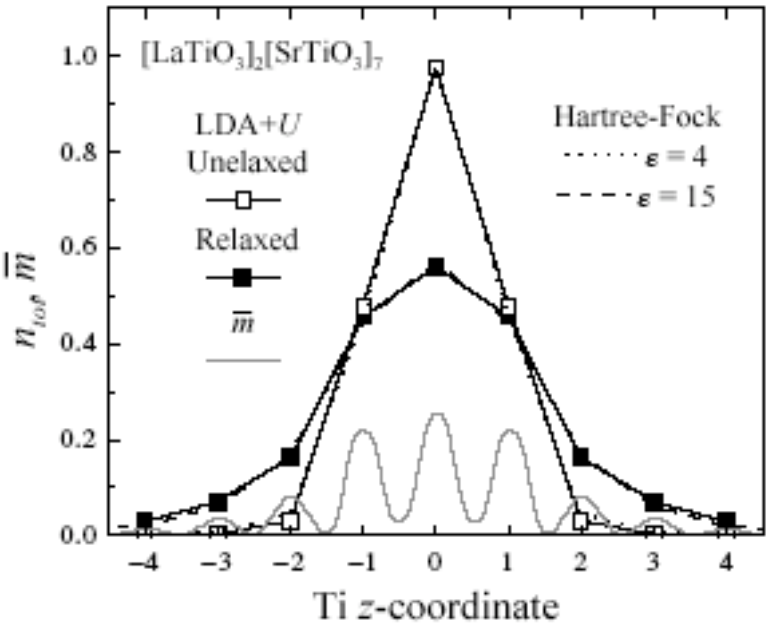
Compare model and LDA+U charge densities





Unrelaxed structure: very well fit by ϵ =4
Relaxed: short length scale ϵ =15--but note slow decay in "far" region

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Message:
for charge density profile

- **Lattice model +dielectric constant is reasonable approximation.**
- **Lattice relaxation modelled by epsilon=15 in STO; smaller in other materials.**
- **Very small, long ranged charge density "tail" missed by this approx.**

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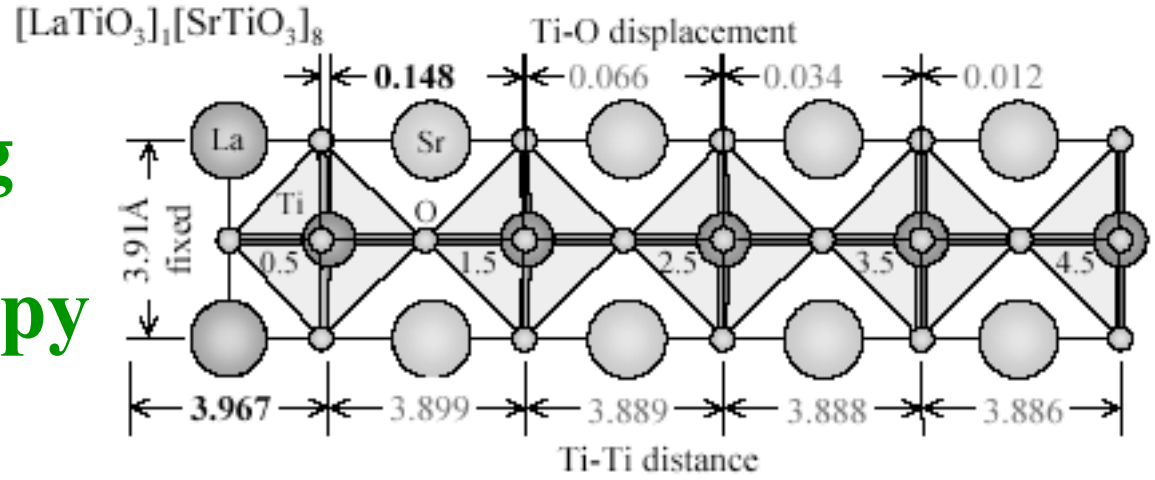
Other effects on electronic physics

- t_{2g} level splitting
- hopping anisotropy



One La Layer: (parameters in eV)

	$t_{xy}^{x,y}$		t_{xz}^{x}		t_{xz}^{z}		ε_{xy}		ε_{xz}	
z_l	–	0.5	–	0.5	−0.5	0.5	–	0.5	–	0.5
1 R	–	0.53	–	0.46	0.44	0.57	–	0.23	–	0.19
1 U	–	0.55	–	0.55	0.56	0.51	–	0.27	–	0.36

Modest hopping anisotropy

Very small crystal field splitting

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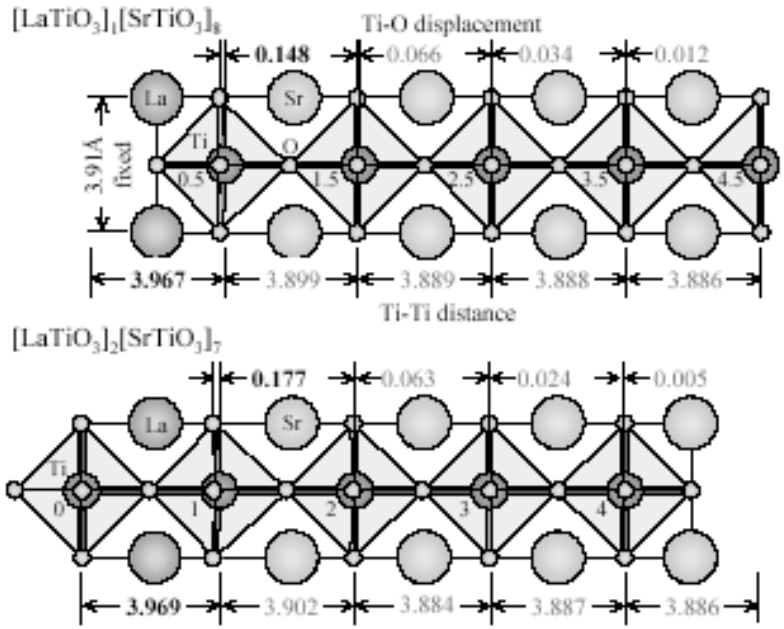
Two La layers: larger effects on hopping



Note: xy-plane hopping of xz/yz orbital decreased

	$t^{x,y}_{xy}$		t^{x}_{xz}		t^{z}_{xz}		ε_{xy}		ε_{xz}	
z_l	–	0.5	–	0.5	−0.5	0.5	–	0.5	–	0.5
1 R	–	0.53	–	0.46	0.44	0.57	–	0.23	–	0.19
1 U	–	0.55	–	0.55	0.56	0.51	–	0.27	–	0.36
z_l	0	1	0	1	0	1	0	1	0	1
2 R	0.63	0.53	0.63	0.38	0.47	0.58	0.66	0.06	0.66	−0.07
2 U	0.63	0.55	0.63	0.5	0.59	0.51	0.66	0.27	0.66	0.36

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Message: anisotropies

- Crystal field splitting small (0.1-0.2eV)
- Big changes: bond lengths, angles
- =>Changes in hopping.
- Largest effect: reduction of in-plane hopping of out of plane orbitals, dxz,dyz

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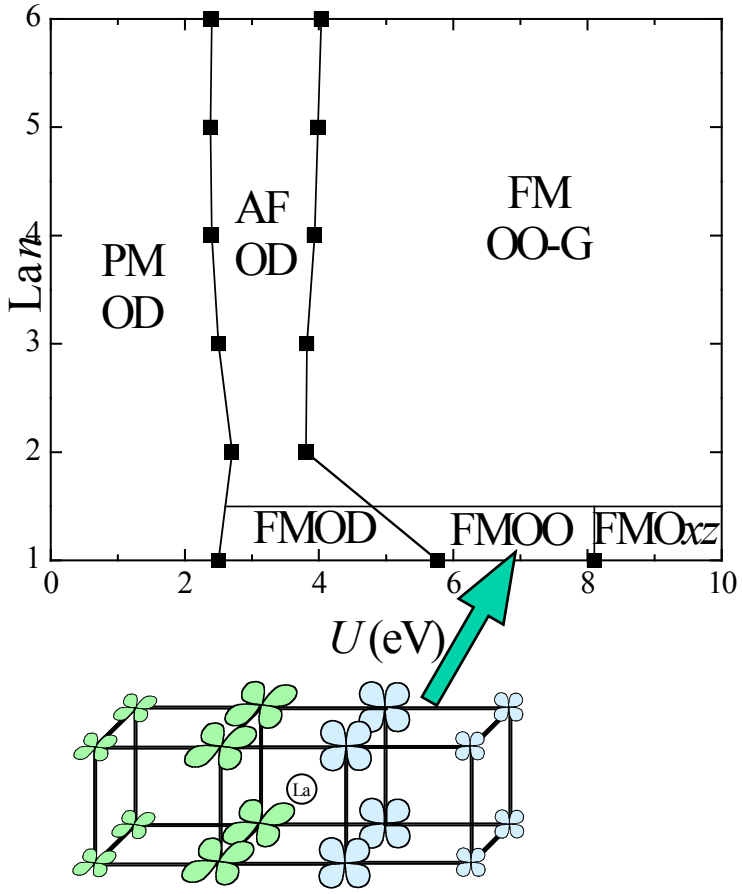
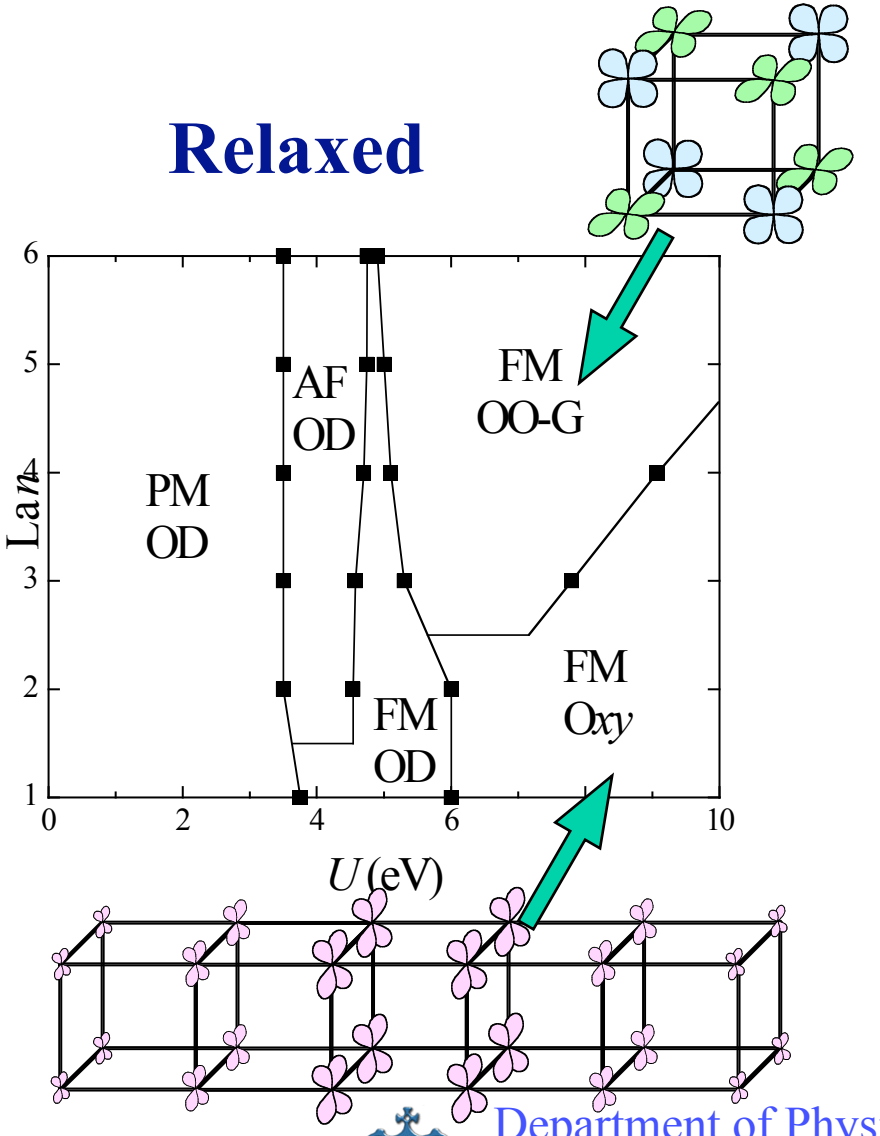
Effect on phase diagram: new phase

Unrelaxed



Relaxed



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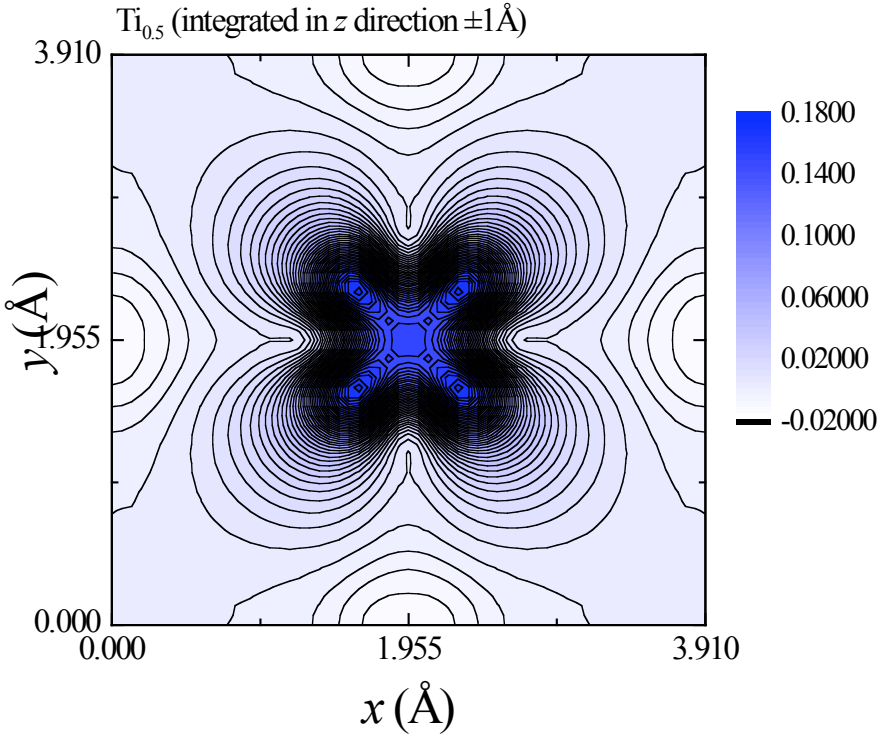
LDA+U: relaxed Structure
Oxy Order

z-integrated Magnetization density: near La; 1 layer structure



Pentcheva PRL 07:
LDA+U => 2 sublattice charge ordering

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Summary: insulator-insulator interfaces

- **0.5 electron at interface, distributed among several layers or subbands=>far from Mott density**
- **Substantial atomic motions**
- **Simple dielectric model of screening reasonable**
  (misses only weak, long-distance "tails" of charge distribution)
- **Main effect of symmetry-breaking: reduction of hopping amplitudes**
- **Predictions (Hartree-Fock; LDA+U): ferromagnetic, ferro-orbital and charge ordering.**

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Summary: insulator-insulator interfaces

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- **Predictions (Hartree-Fock; LDA+U): ferromagnetic, ferro-orbital and charge ordering.**

?Are the predictions right?

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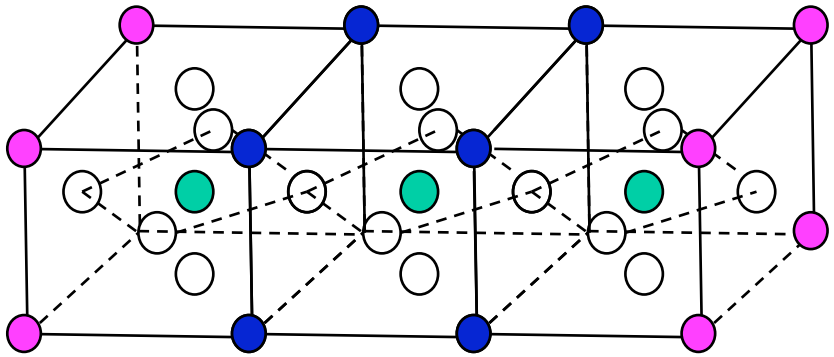
$(AA')BO_3(001)$ Superlattice ($LaTiO_3/SrTiO_3$)



: Ti (B)

: Sr (A)

: La (A')

: O

Lattice Model:

*Define heterostructure: charge +1 at La site 0 at Sr

*Electrons: move among B (Ti) sites

*Charge distribution: discrete Poisson equation

*?many body physics on correlated B site?

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Interactions:

- **Long ranged coulomb: Hartree=>self consistent on-site potential**

$$V(R_i) = -\sum_j \frac{e^2}{\epsilon \left| \vec{R}_i - \vec{R}_j^A \right|} + \sum_{j,\sigma} \frac{e^2 < n_{j,\sigma} >}{\epsilon \left| \vec{R}_i - \vec{R}_j \right|}$$

- **On site: Hartree**

$$\Sigma(r, r'; \omega) \rightarrow \left[\Sigma_{Hartree}(r) + V(r)\right] \delta(r - r')$$

- **or dynamical mean field**

$$\Sigma(r, r', \omega) \rightarrow \left[\Sigma_{DMFT}(r, \omega) + V(r)\right] \delta(r - r')$$

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Dynamical Mean Field I

Metzner/Vollhardt; Mueller Hartmann **KOTLIAR**

- **Many-body theory=>exists functional F of self energy**

$$F[\{\Sigma(r,r',\omega)\}] = F_{univ}[\{\Sigma(r,r',\omega)\}]$$
$$+Tr\left[ln\left(G_0^{-1}(r,r',\omega) - \Sigma(r,r',\omega)\right)\right]$$

extremized at correct self energy and from which ALL RESPONSE FUNCTIONS can be extracted.

- **Kotliar: there exists tractable and ?accurate? approximation**

$$\Sigma(r,r',\omega) \rightarrow \Sigma(r,r,\omega)$$

and 'convenient' procedure for doing minimization

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Dynamical Mean Field: II

$$F[\{\Sigma(r,r',\omega)\}] \rightarrow \sum_{r_i} F_{approx}[\{\Sigma(r_i,\omega)\}]$$
$$+Tr\left[ln\left(G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right)\right]$$

- **F_{approx}: functional of one function of frequency <=> "quantum impurity (QI) model" (one for each lattice site)**

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Dynamical Mean Field: II

$$F[\{\Sigma(r,r',\omega)\}] \rightarrow \sum_{r_i} F_{approx}[\{\Sigma(r_i,\omega)\}]$$
$$+Tr\left[ln\left(G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right)\right]$$

- **F_{approx}: functional of one function of frequency <=> "quantum impurity (QI) model" (one for each lattice site)**
- **Extremum condition: self consistency equation**

$$\frac{\delta F_{approx}}{\delta \Sigma(r,\omega)} \equiv G_{QI}(r,\omega) = \left[G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right]^{-1}_{r \rightarrow r'}$$

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Dynamical Mean Field: II

$$F[\{\Sigma(r,r',\omega)\}] \rightarrow \sum_{r_i} F_{approx}[\{\Sigma(r_i,\omega)\}]$$
$$+Tr\left[ln\left(G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right)\right]$$

- **F_{approx}: functional of one function of frequency <=> "quantum impurity (QI) model" (one for each lattice site)**
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$$\frac{\delta F_{approx}}{\delta \Sigma(r,\omega)} \equiv G_{QI}(r,\omega) = \left[G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right]^{-1}_{r \rightarrow r'}$$

'Quantum Impurity Model': 0+1 d field theory tractable (marginally) by numerical simulation (quantum monte carlo)

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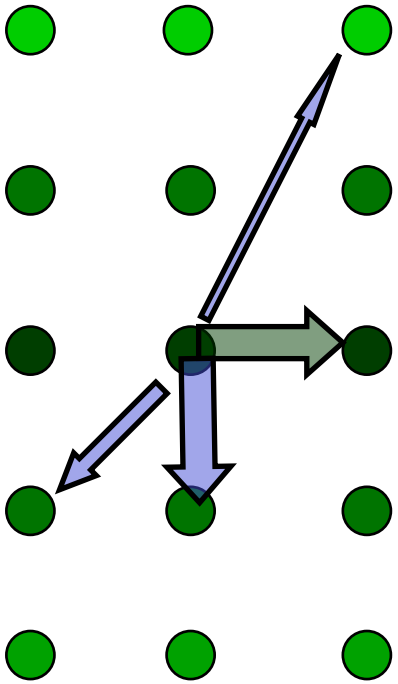
Dynamical Mean Field III

$$\frac{\delta F_{approx}}{\delta \Sigma(r,\omega)} \equiv G_{QI}(r,\omega) = \left[G_0^{-1}(r,r',\omega) - \Sigma(r,\omega)\right]^{-1}_{r\to r'}$$



Self-consistent embedding interp: F_{approx}==’free energy’ of ‘impurity’ coupled to ‘bath’ determined by nearby sites (couplings fixed by band structure). Extremum condition <=> consistency between ‘bath’ and self energy on each site.

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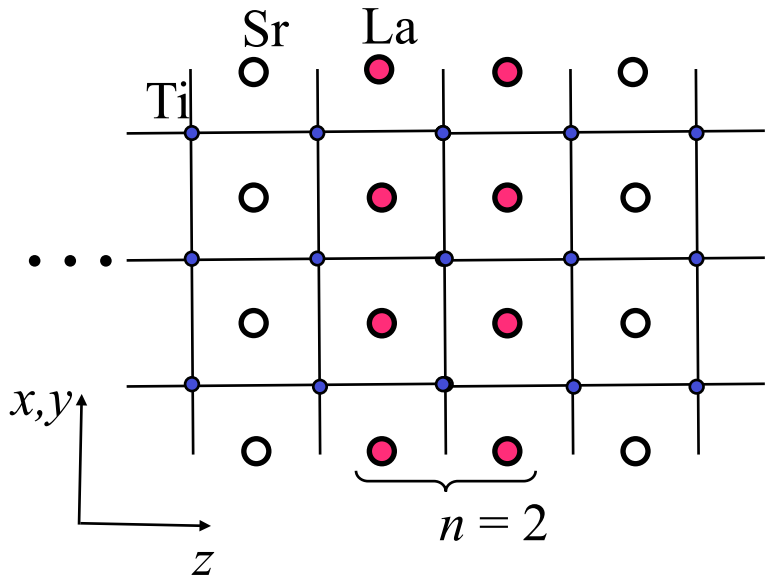
Dynamical Mean Field for Heterostructure: General Remarks

Variables:

transverse coordinate z

in-plane (xy) wavevector k



Easier case: in-plane translation invariance (FM, layer AF)

G->G(k,z,z';w)

Harder: in-plane AF:

G->G(k,k+Q;z,z';w)

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DMFT Formalism
In-plane translational invariance

$$G_z^{imp}(\omega) = \int \frac{d^2 k_{\|}}{(2\pi)^2} G_{zz}^{latt}(k_{\|},\omega)$$

$$\hat{G}_{zz'}^{latt}(k_{\|},\omega) = \begin{bmatrix} \alpha_1 & t & & & \\ t & \alpha_2 & t & & \\ & t & \ddots & & \\ & & & \ddots & t \\ & & & t & \alpha_N \end{bmatrix}^{-1}$$

Layers coupled.
must solve 1 impurity model for each layer
<u>and</u> self-consistently obtain charge density

$a_z = \omega + \mu - \varepsilon_{k\|} - V_z - \Sigma_z(\omega)$

$\varepsilon_{k\|}$: in-plane dispersion

V_z : potential from long-ranged Coulomb

N: total layer #

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DMFT Formalism
In-plane antiferromagnetism

$$G^{imp}_{zA(B)}(\omega) = \int \frac{d^2 k_{\|}}{(2\pi)^2} G^{latt}_{zA(B),zA(B)}(k_{\|},\omega)$$

$$\hat{G}^{latt}_{zz'}(k_{\|},\omega) = \begin{bmatrix} \alpha_{1A} & t & & & -\varepsilon_{k\|} & & & \\ t & \alpha_{2A} & t & & & -\varepsilon_{k\|} & & \\ & t & \ddots & t & & & \ddots & \\ & & t & \alpha_{NA} & & & & -\varepsilon_{k\|} \\ -\varepsilon_{k\|} & & & & \alpha_{1B} & t & & \\ & -\varepsilon_{k\|} & & & t & \alpha_{2B} & t & \\ & & \ddots & & & t & \ddots & t \\ & & & -\varepsilon_{k\|} & & & t & \alpha_{NB} \end{bmatrix}^{-1}$$

2 sublattice Neel: must solve 2 impurity models for each layer. Also matrix inversion non-trivial (basis which diagonalizes layer dep on k,w and layer)

$$a_{zA(B)} = \omega + \mu - V_z - \Sigma_{zA(B)}(\omega)$$

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Final complication many orbitals=> need full (Slater-Kanamori) interaction

$$H_{int} = U \sum_a n_{ja\uparrow} n_{ja\downarrow} + (U' - J) \sum_{a>b,\sigma} n_{ja\sigma} n_{jb\sigma}$$
$$+U' \sum_{a \neq b} n_{ja\uparrow} n_{jb\downarrow} + J \sum_{a \neq b} d^\dagger_{ja\uparrow} d_{jb\uparrow} d^\dagger_{jb\downarrow} d_{ja\downarrow}$$
$$+J' \sum_{a \neq b} d^\dagger_{ja\uparrow} d^\dagger_{ja\downarrow} d_{jb\downarrow} d_{jb\uparrow}$$

Computational expense ~$2^{n_{orbital}}$

Methods now in hand to treat this.

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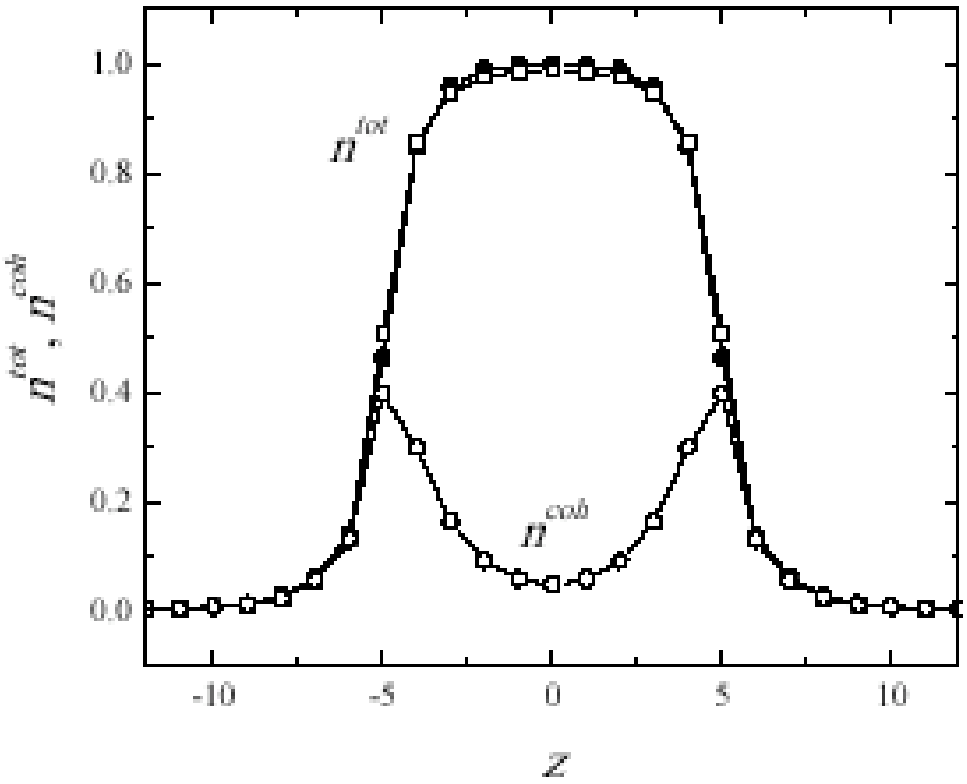
Density profile independent of method used to compute it (within reason)



● Hartree-Fock

○ DMFT

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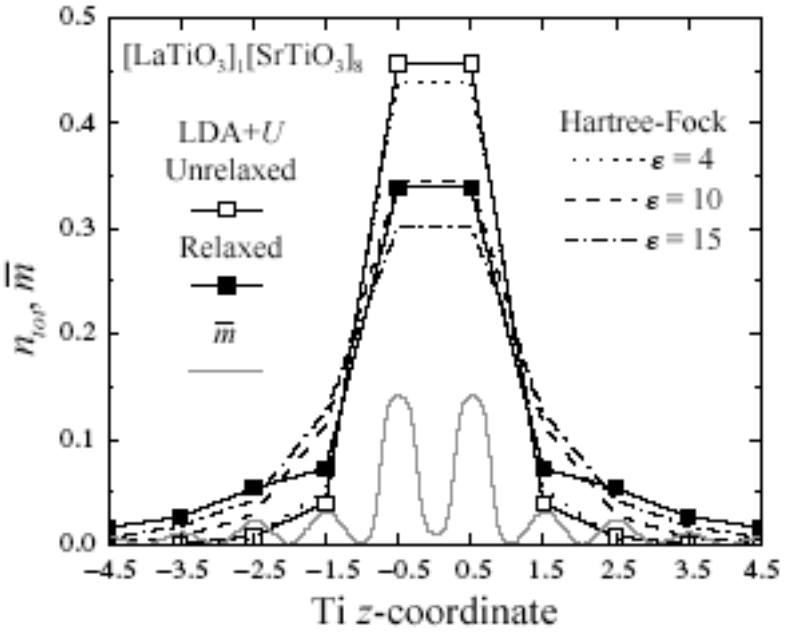
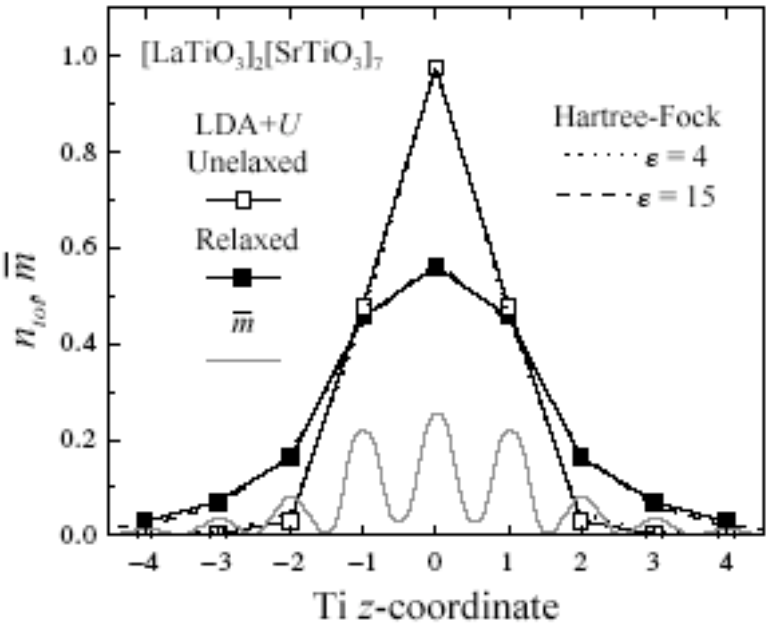
Compare model and LDA+U charge densities





Unrelaxed structure: very well fit by ϵ =4
Relaxed: short length scale ϵ =15--but note slow decay in "far" region

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Charge profile:
~3 unit cell wide 'metallic edge'

Examine edge excitations in more detail

Important object: layer resolved spectral function (observable in principle in photoemission)

$$A(z,z;k,\omega) = lim_{z' \to z} \frac{1}{\pi} ImG(z,z';k,\omega)$$

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Layer Spectral Function

n=10 layer Hubbard heterostructure

U=16t>U $_c$ ~14.7t

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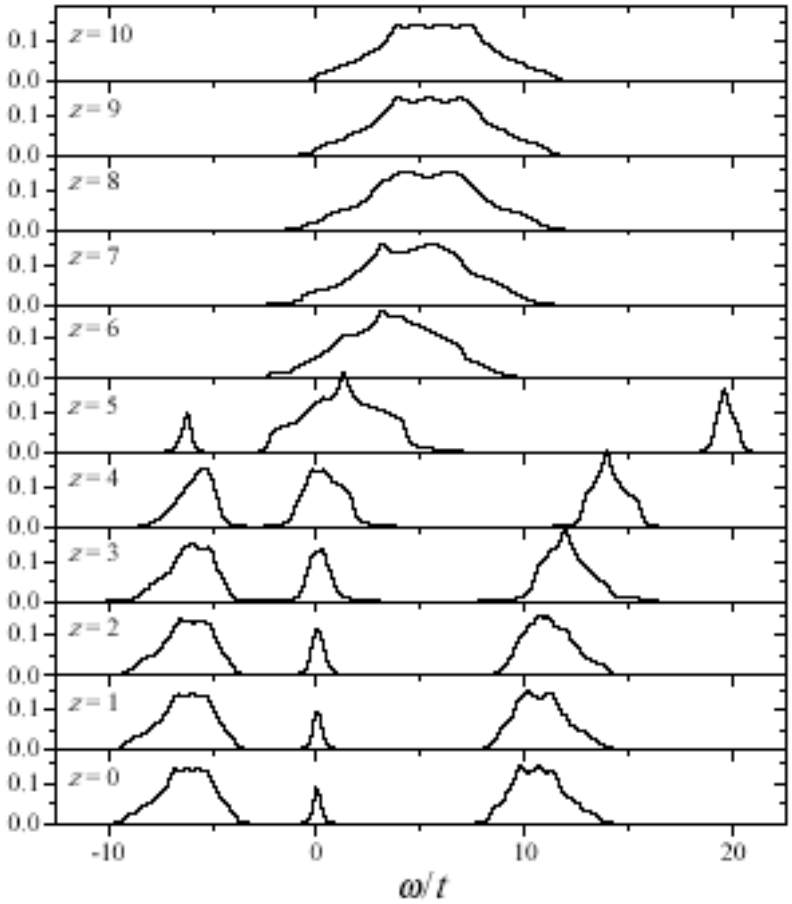
Layer Spectral Function

n=10 layer Hubbard heterostructure

U=16t>U ~14.7t



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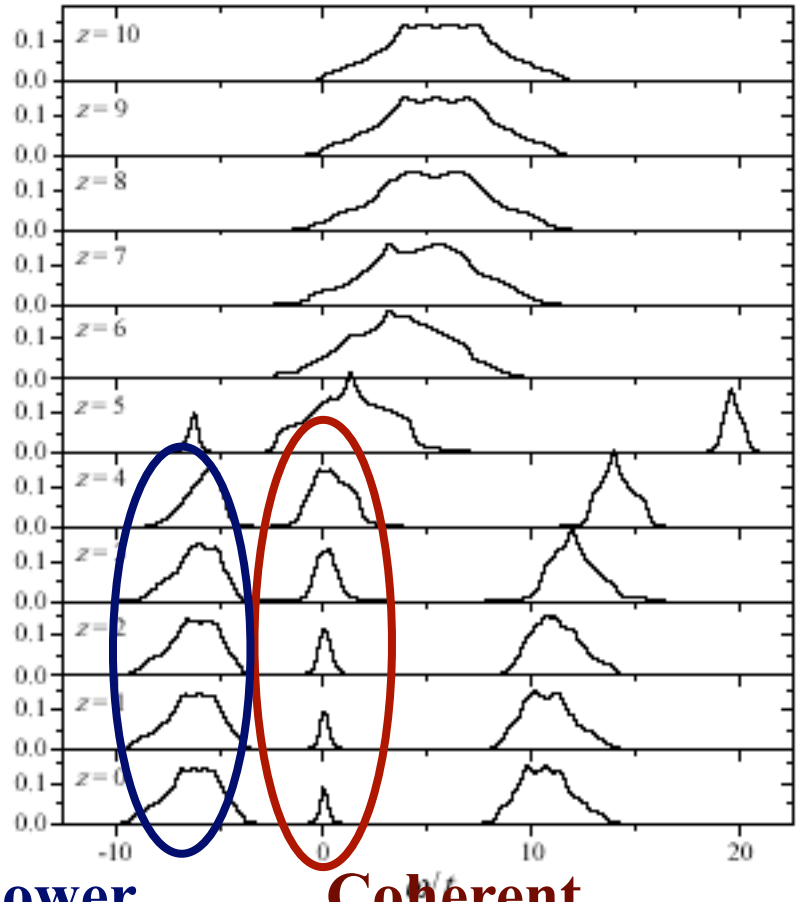
Layer Spectral Function

n=10 layer Hubbard heterostructure

U=16t>U ~14.7t



Lower Hubbard band

Coherent quasiparticle

Note: spectrum in intermediate region is not exactly superposition of spectral of Mott and band insulators

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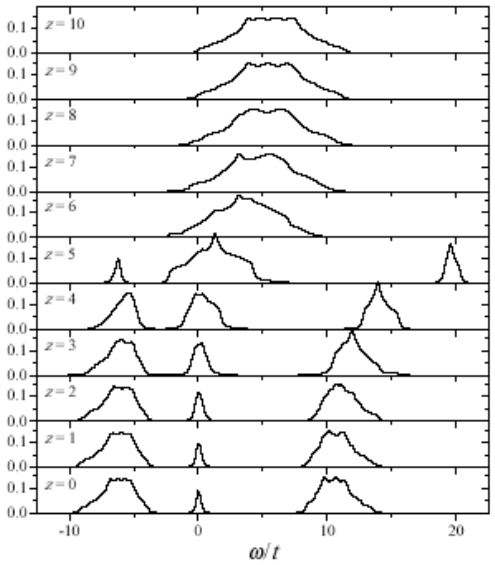
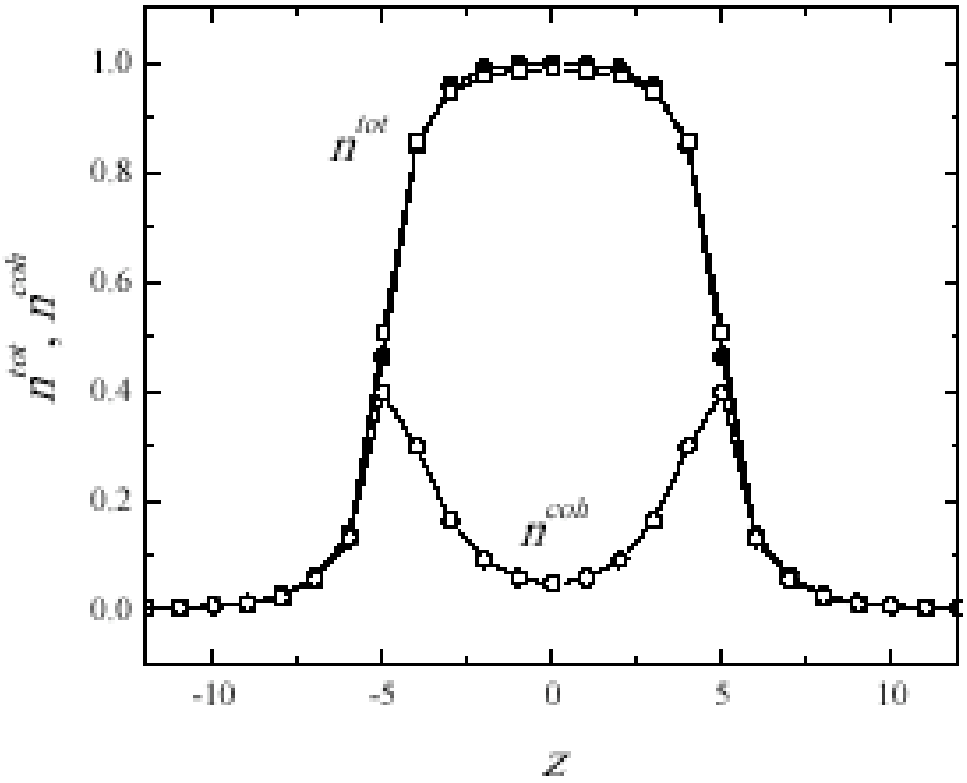
Density profile independent of method used to compute it (within reason)





● Hartree-Fock

○ DMFT

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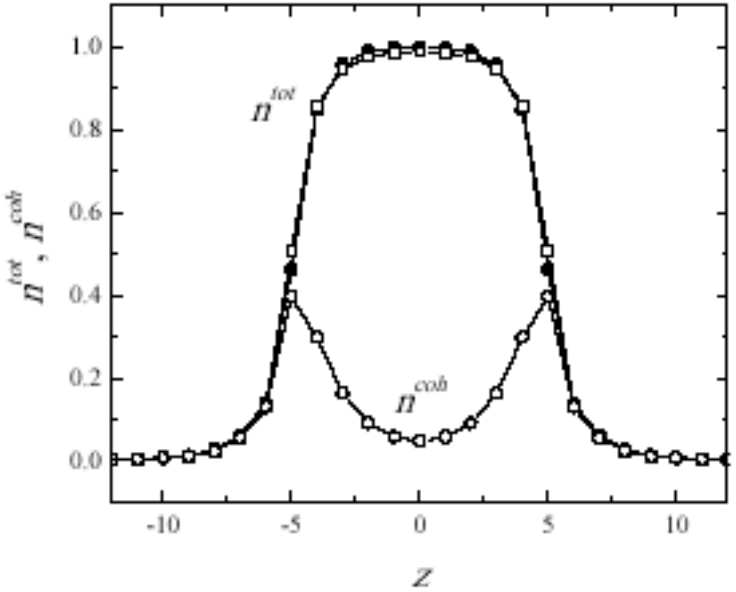
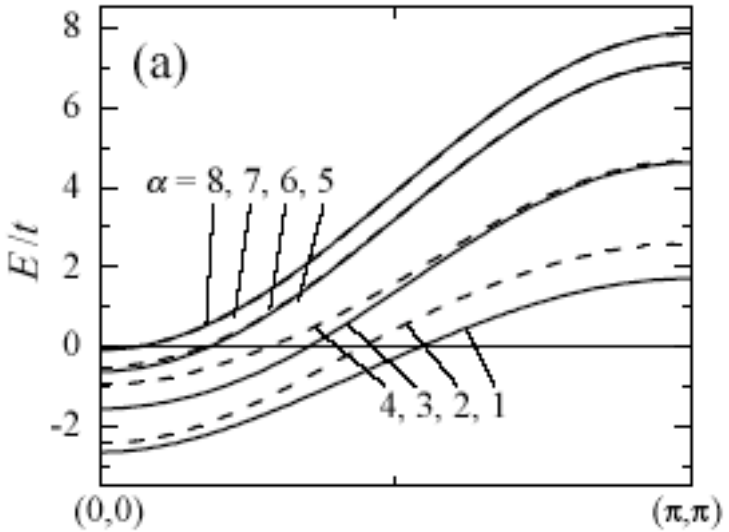
Edge states: closer study

Coherent particles: concentrated near edge



coherent quasiparticle bands



moderately correlated (Z or m*/m ~2-3)

Metallic behavior only from coherent qp

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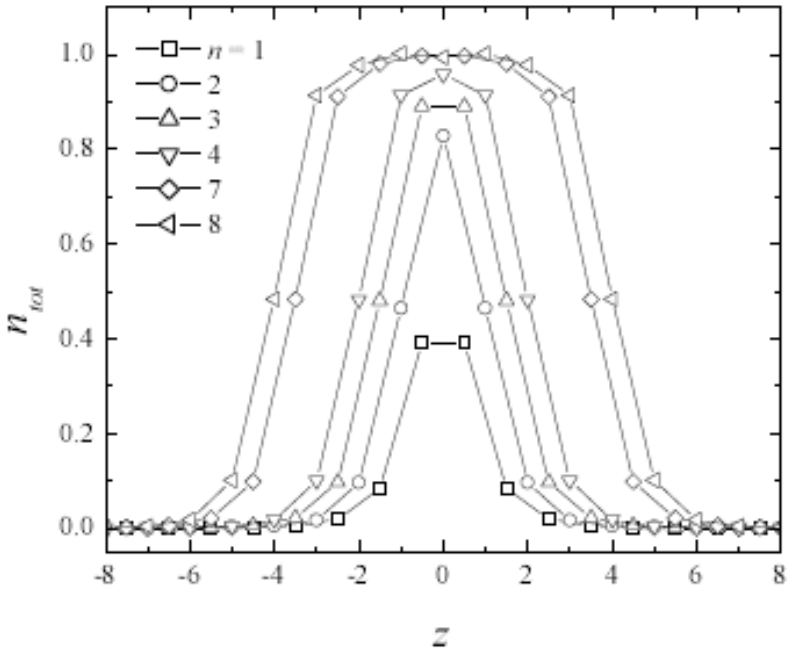
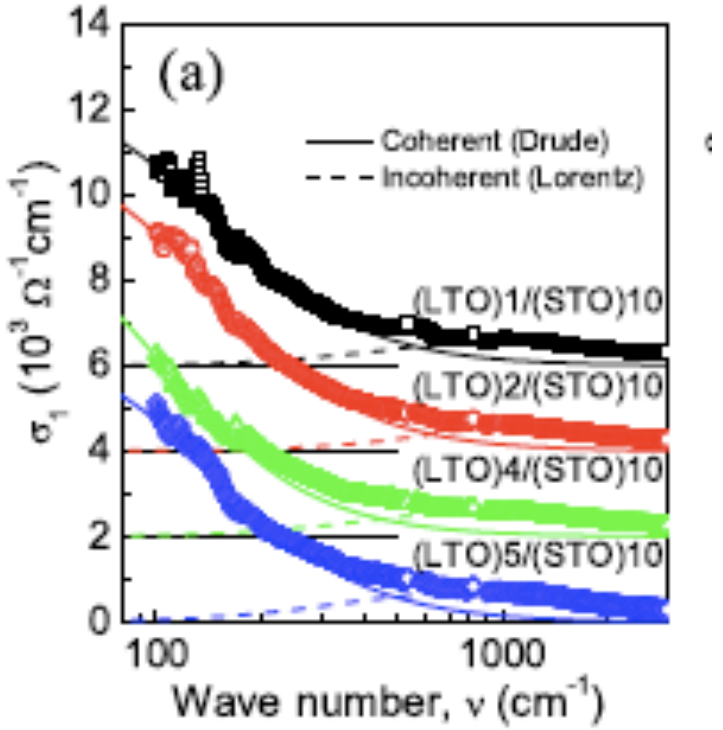
3 unit cell edge





Calculation:
#layers<5, conductivity ~#La
#layers >5, cond ~ # interfaces

Expt: cond indep #La, #int

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Summary: 'Hubbard' Mott insulator/ band insulator heterostructures

- ~3 unit cell wide transition region
- supports metallic behavior
- 'metallic edge' moderately correlated
- Question: does 'edge' support new magnetic (or superconducting?) behavior
- expt, theory not (yet?) consistent

See Okamoto/Millis Phys. Rev. B72, 235108 (2005)

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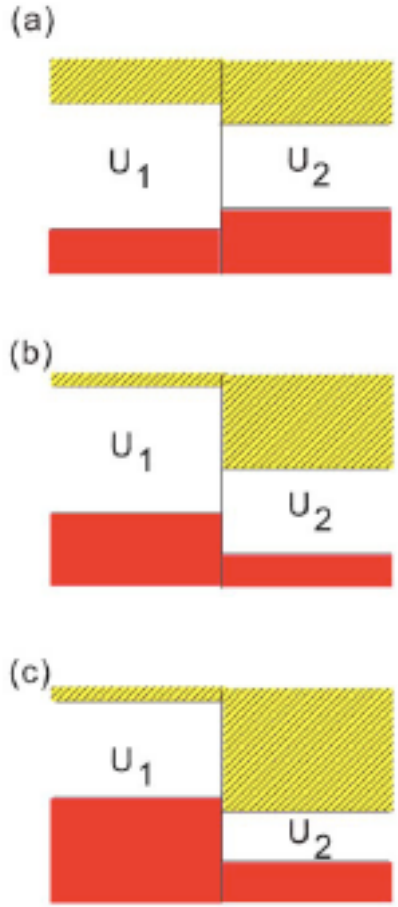
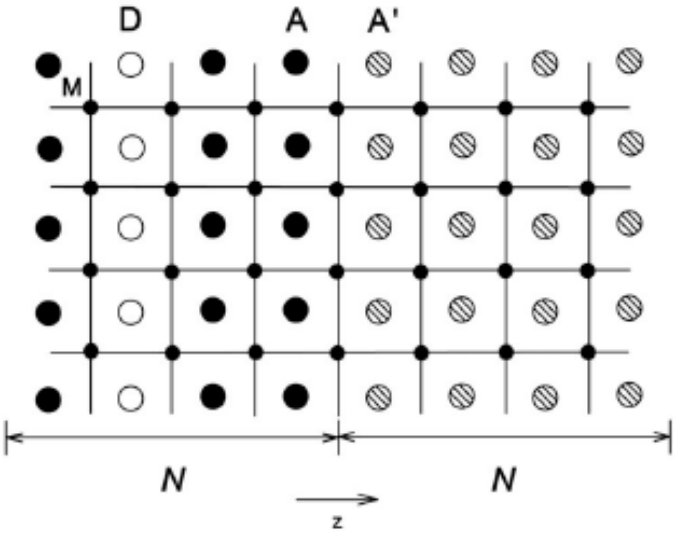
Lee/McDonald: Mott-Mott structures

Possible band alignments



they study: type (a) with row of dopants in 1



PHYSICAL REVIEW B 74, 075106 (2006)

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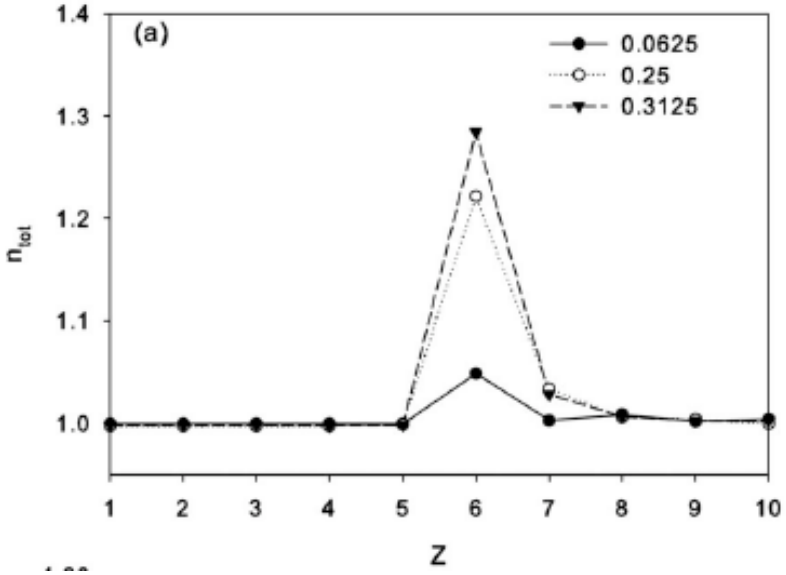
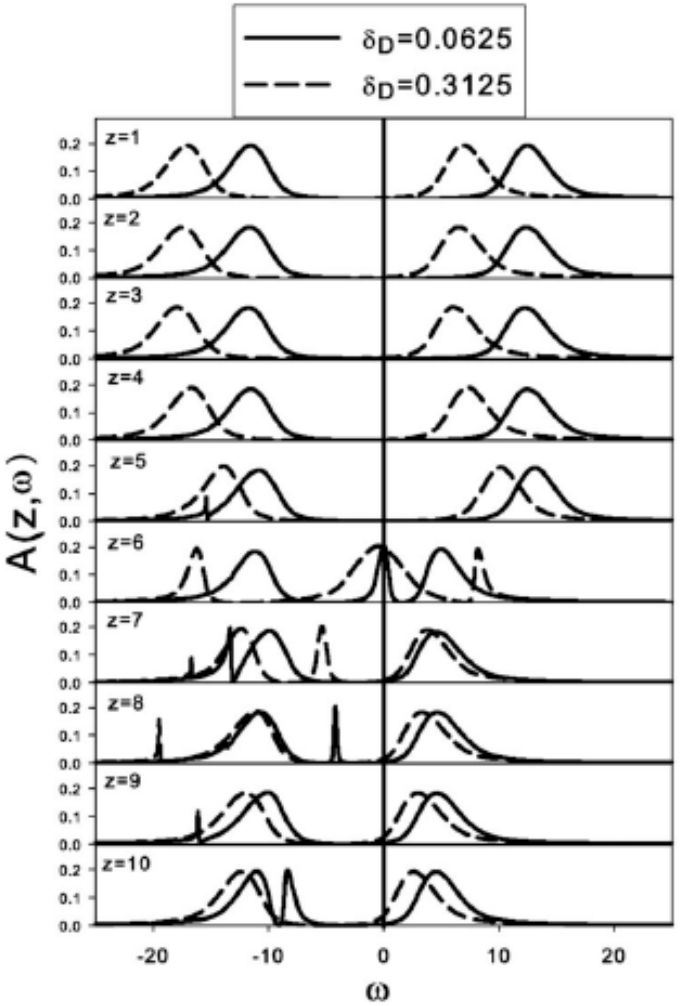
Results





Lightly doped state on small gap side of interface

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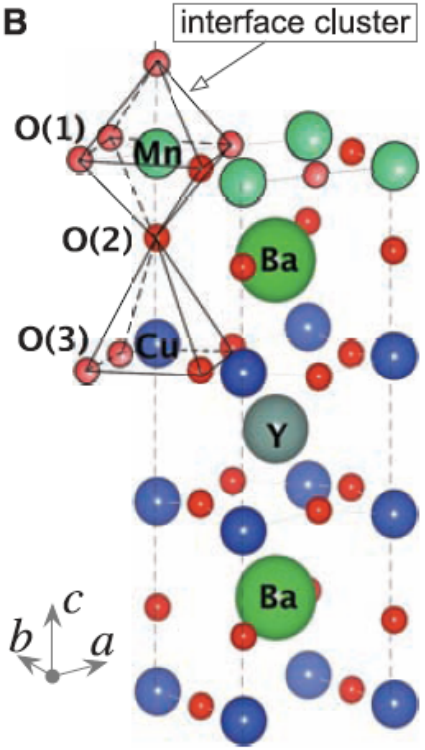
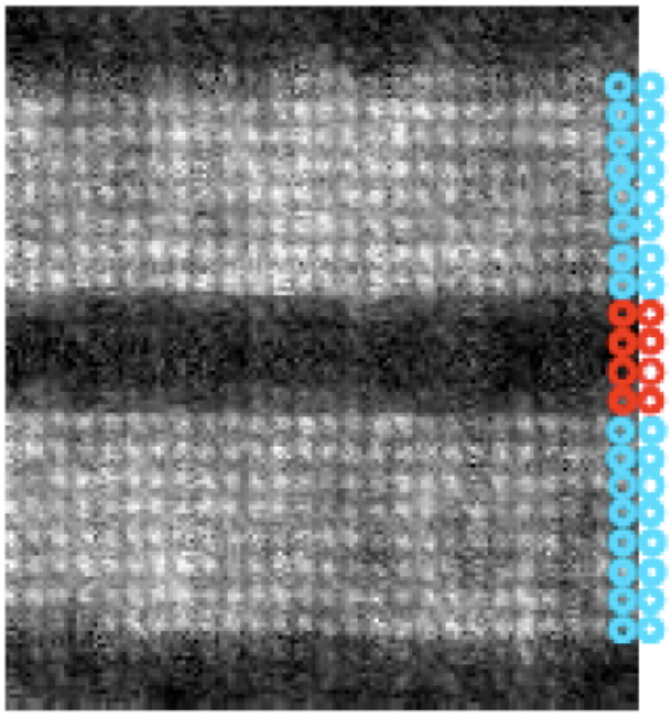
Competing orders

$LaMnO_3/YBa_2Cu_3O_7$



Chakhalian 06

$(LaMnO_3)_8/(SrMnO_3)_4$



Bhattacharya...Eckstein 08

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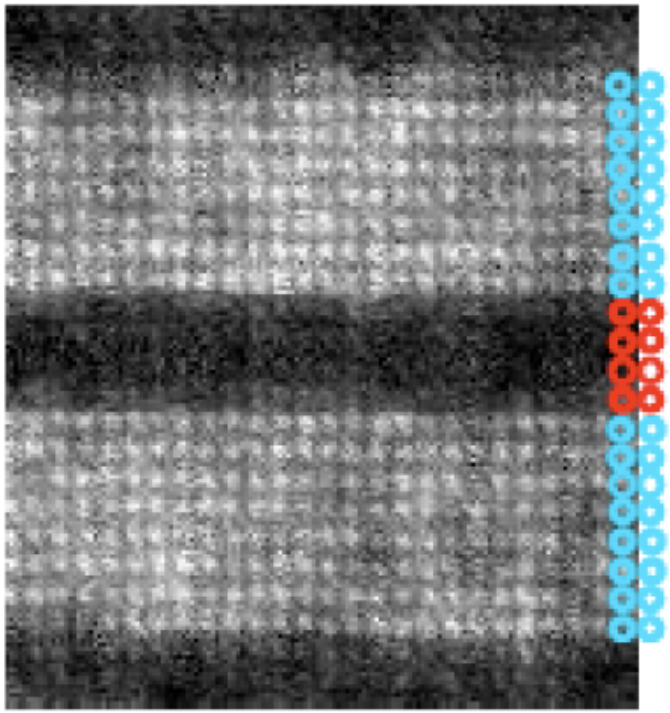
Easier case

$(LaMnO_3)_8/(SrMnO_3)_4$



Bhattacharya...Eckstein 08

Homometallic. Physics basically understood

$LaMnO_3$: 1 mobile electron/site;
orbital order;
A-type AF (layered FM)

$SrMnO_3$: no mobile electrons;
no orbital order;
G-type AF (3d Neel)

=>2 kinds of order to play with

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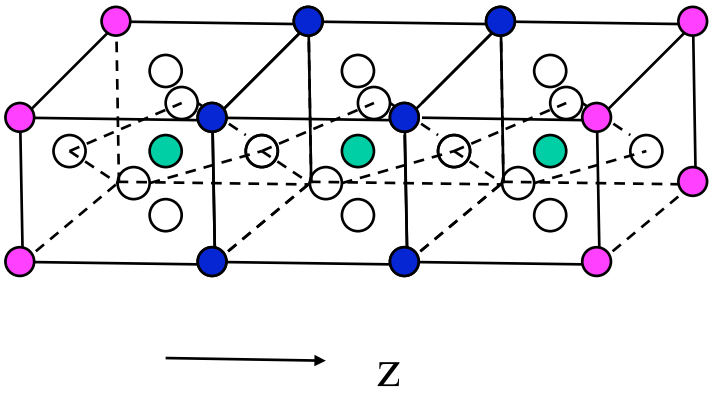
Magnetic physics: each Mn has S=3/2 "core spin"



: Mn
: Sr
: La
: O

Layer (m,n)= m La n Sr (here (2,1))

Interaction: "double-exchange"

$$H = -\sum_{i\delta ab\sigma} t^{ab}(\delta)\left(d^{\dagger}_{i+\delta a\sigma} d_{ib\sigma} + H.c.\right) + J\sum_{i} \vec{S}_i \cdot \left(d^{\dagger}_{ia\alpha}\sigma_{\alpha,\beta} d_{ia\beta}\right)$$

+ potential from La/Sr and n(r) as before.

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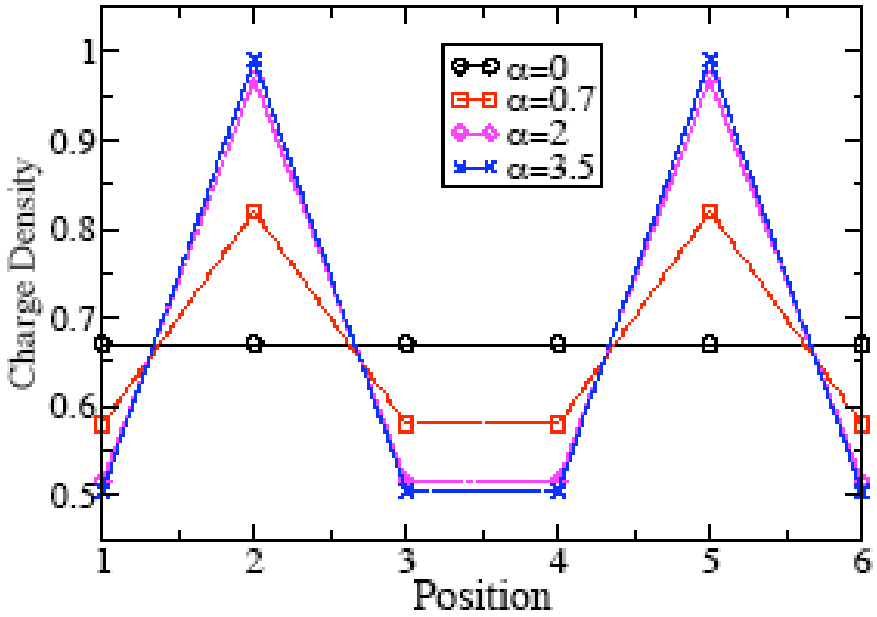
Key physics: binding of charge to La layers

Parameter: ratio of coulomb interaction to hopping (for physical a, bandwidth=3.6eV)

$$\alpha = \frac{e^2}{\epsilon a t} \approx \frac{10}{\epsilon}$$

(2 La, 1 Sr)



$\alpha \geq 2$ Complete binding of charge to near-La layers

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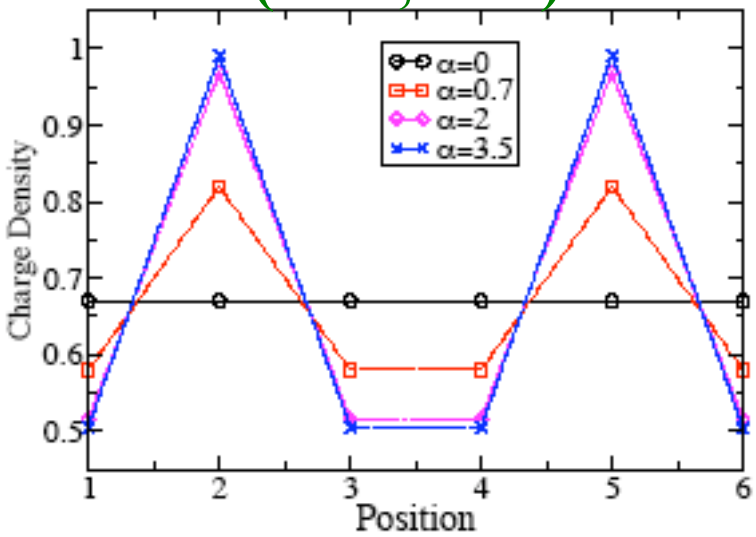
Near Tc:
2 magnetic phases:

Layer (1,2)				
	$T_c(t)$	n_A	n_B	$m_A : m_B$
$\alpha = 0.7$	0.105	0.206	0.09	1.68 :1
$\alpha = 3.5$	0.103	0.249	0.009	6.27:1
Layer (2,1)				
$\alpha = 0.7$	0.085	0.29	0.41	5.66:1
$\alpha = 3.5$	0.101	0.25	0.5	-9.45:1

(2 La, 1 Sr)



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	$T_c(t)$	n_A	n_B	$m_A : m_B$
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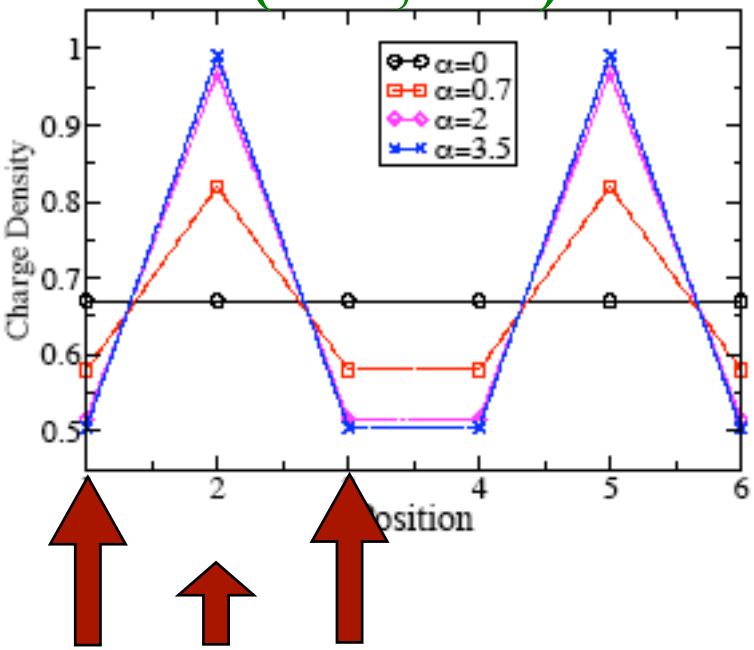
(2 La, 1 Sr)



Weaker binding (a<2): ferromagnet (FM)

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Near Tc:
2 magnetic phases:

Layer (1,2)				
	$T_c(t)$	n_A	n_B	$m_A : m_B$
$\alpha = 0.7$	0.105	0.206	0.09	1.68 :1
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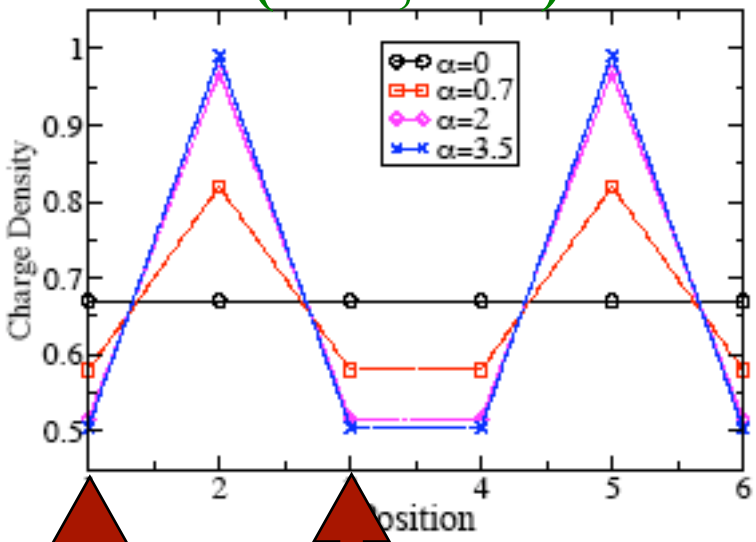
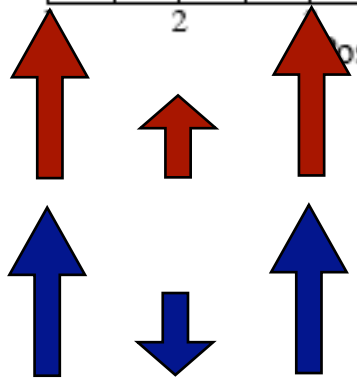
(2 La, 1 Sr)





Weaker binding (a<2): ferromagnet (FM)

Stronger binding (a>2): layer-ferromagnet (LFM)

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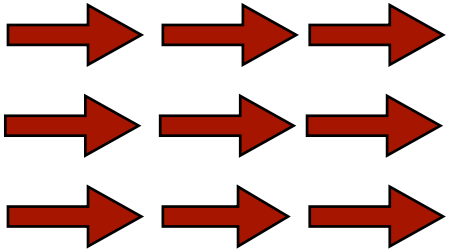
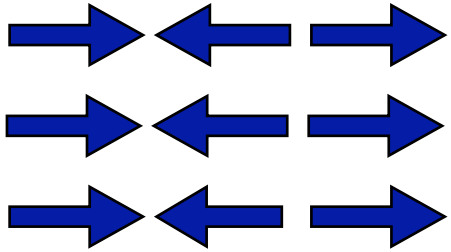
More generally: 3 solutions

La La

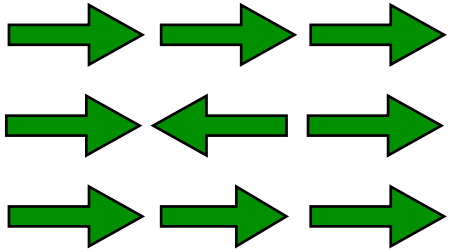
*Ferromagnetic



*‘Layer Ferro”



*AF Core



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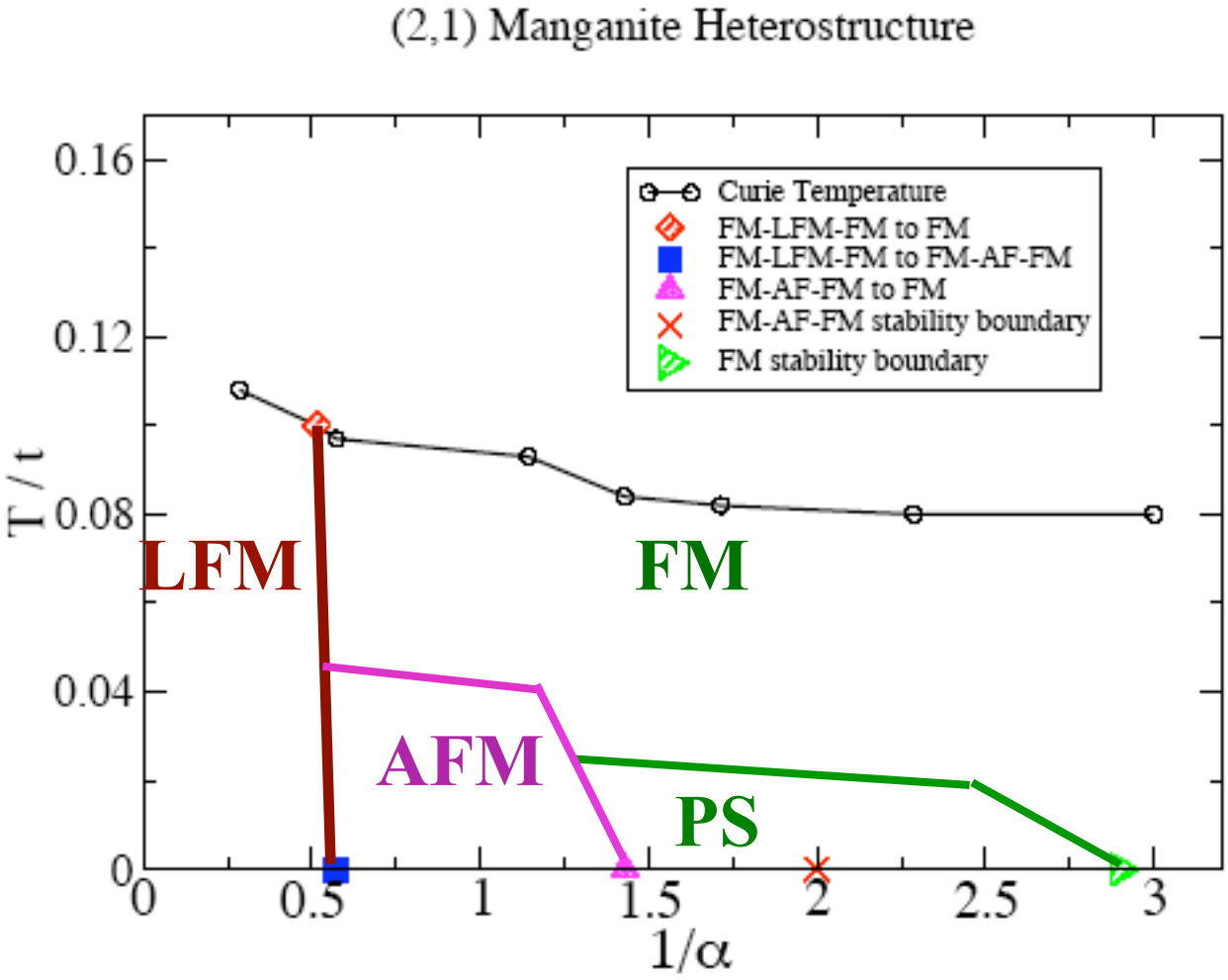
Calculated Phase Diagram:
(label by order on central layer)



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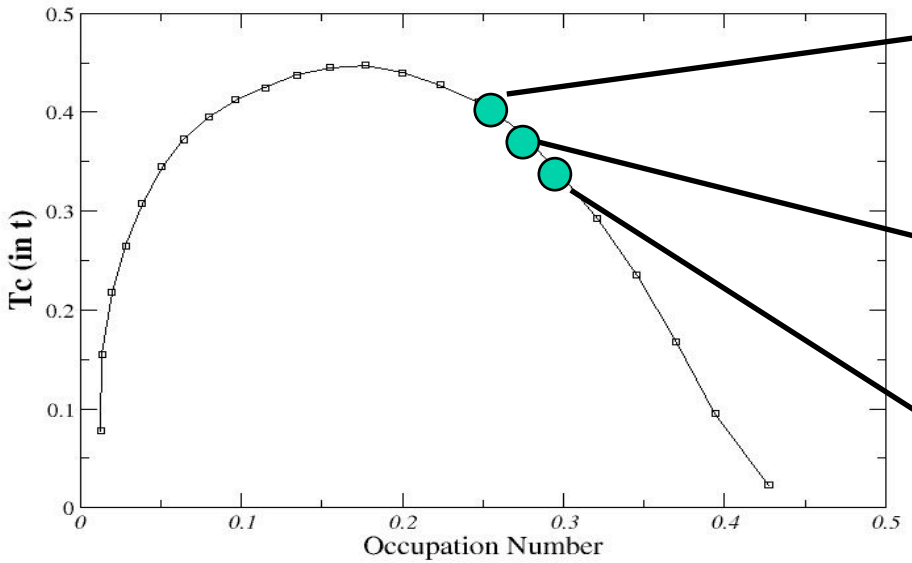
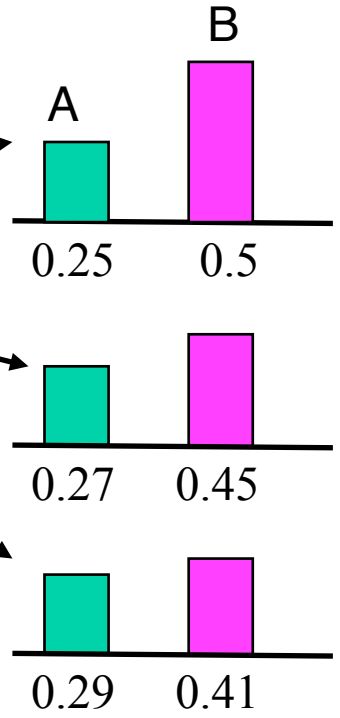
Tc vs Bulk Tc

(note: for relevant J, 2D and 3D bulk almost identical)

Bulk Tc



Heterostructure results



1/a= 0.34
Tc~0.106

1/a=0.83
Tc~0.-95

1/a= 1.4
Tc~0.085

!! dependence of Tc on **a** understood from bulk phase diagram.

B site: almost completely full – almost no contribution to Tc.

density at A site determines Tc!

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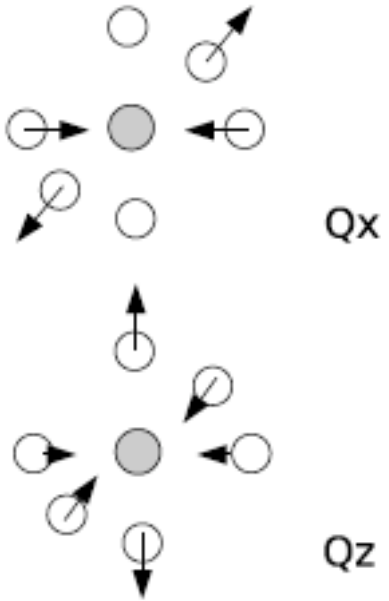
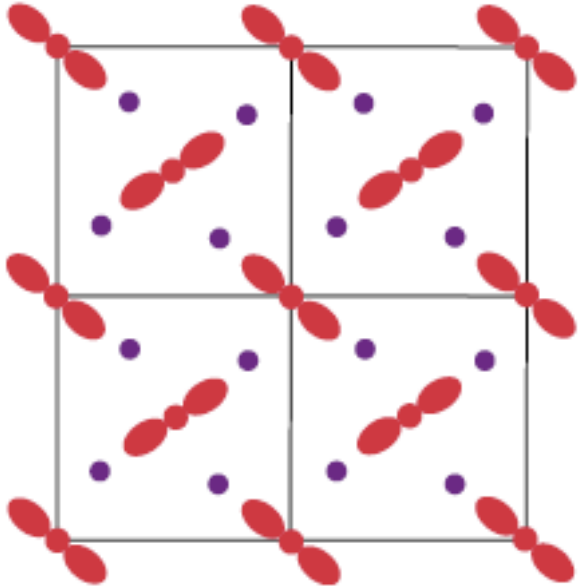
Real manganites: cooperative orbital (Jahn Teller) order

Local volume-preserving lattice distortions





Each O is shared between 2 Mn, so distortion on one site propagates to others

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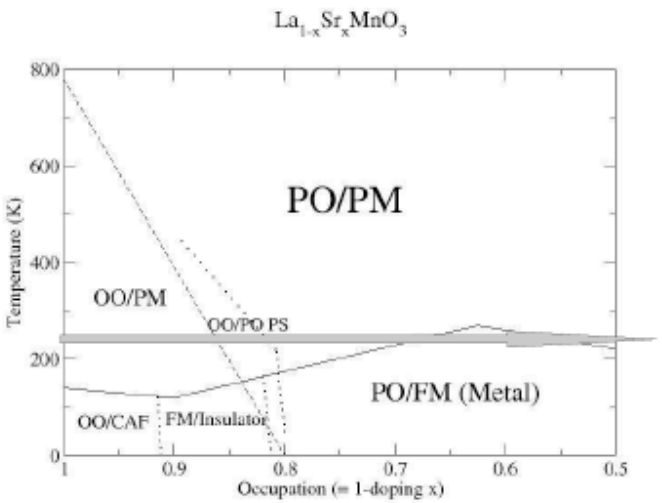
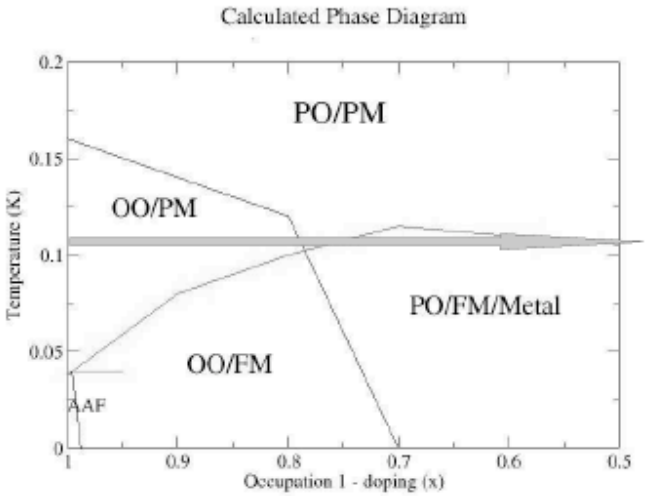
Calculation vs Expt: bulk

Expt



Calc



Calculation underestimates OO T_c
Overestimates doping regime of orbital order
Overestimates magnetic T_c

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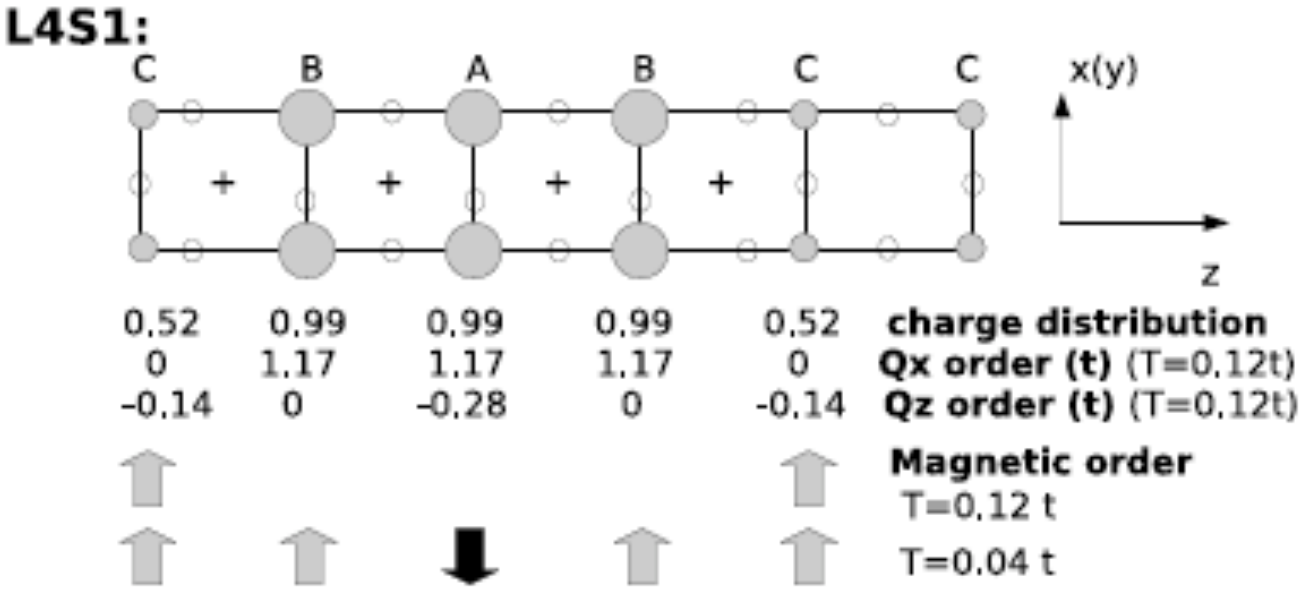
Superlattice: model calculations



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Result: "Chungwei's rules"

- **Charge distribution determined by screening; essentially independent of electronic phase**

- **Orbital order only weakly coupled between layers; determined by bulk behavior at layer density**

- **Layers are ferromagnetically coupled unless density >0.95**

- **In plane conductivity: each layer has conductivity equal to bulk conductivity appropriate to its density; layers add in parallel**

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Bulk vs averaged DL conductivity

α	0.3	0.09	0.3	0.09	0.3	0.09
$\bar{\sigma}_{xx}^{bulk}$	0.083	0.115	0.064	0.093	0.58	0.082
σ_{xx}^{SL}	0.077	0.105	0.067	0.093	0.6	0.081
SL	L2S1	L2S1	L3S1	L3S1	L4S1	L4S1

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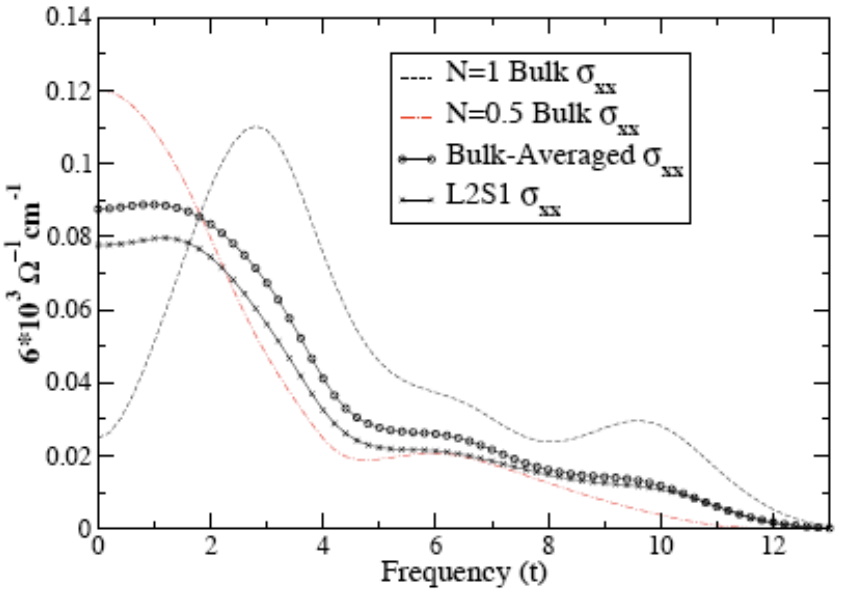
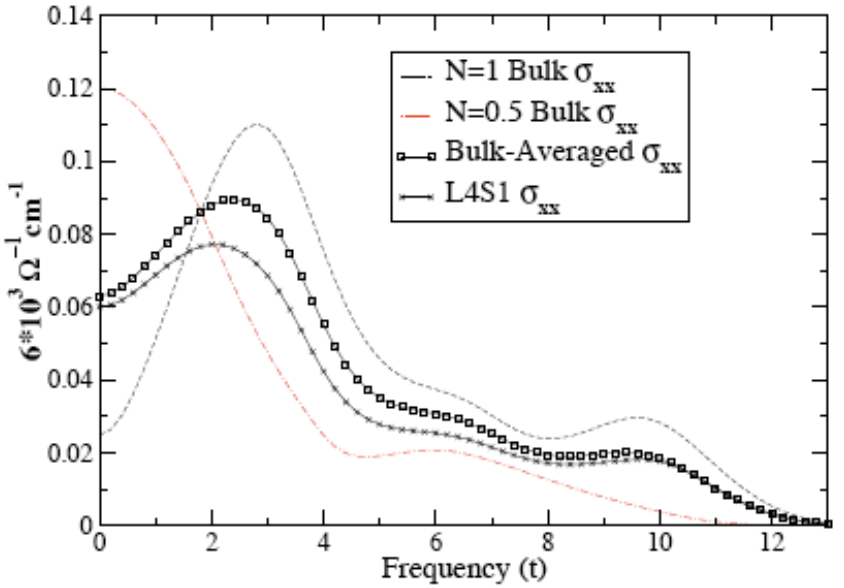
Optical conductivities also average





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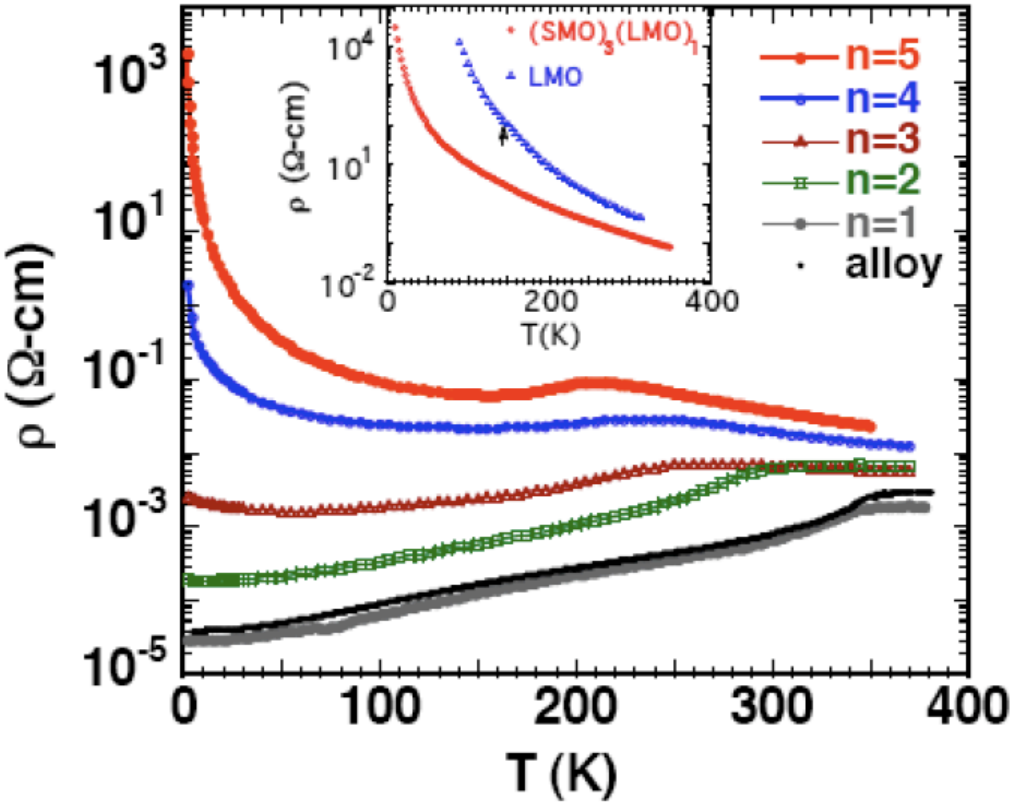
Not consistent with experiment

$(LaTiO_3)_{2n}/(SrTiO_3)_n$



Waruswithana et al (UIUC)

Theory: rho ~ n

Expt: Log[rho] changes fast with n

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Summary

Homometallic superlattices: all you really need to know is the charge density profile and the bulk phase diagram

Agreement bet. expt and theory not (yet) great

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What the field needs now

- **Identify "hydrogen atom" of heterostructures:**
  simple enough to create and study; rich enough to reveal new properties Not found in bulk of either constituent

- **Undertake systematic comparisons:**
  - **materials processing <=> properties**
  - **growth <=> defects**
  - **control (gating) <=> properties**
  - **experiment<=>theory**

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