

Electronic reconstruction in manganite heterostructures

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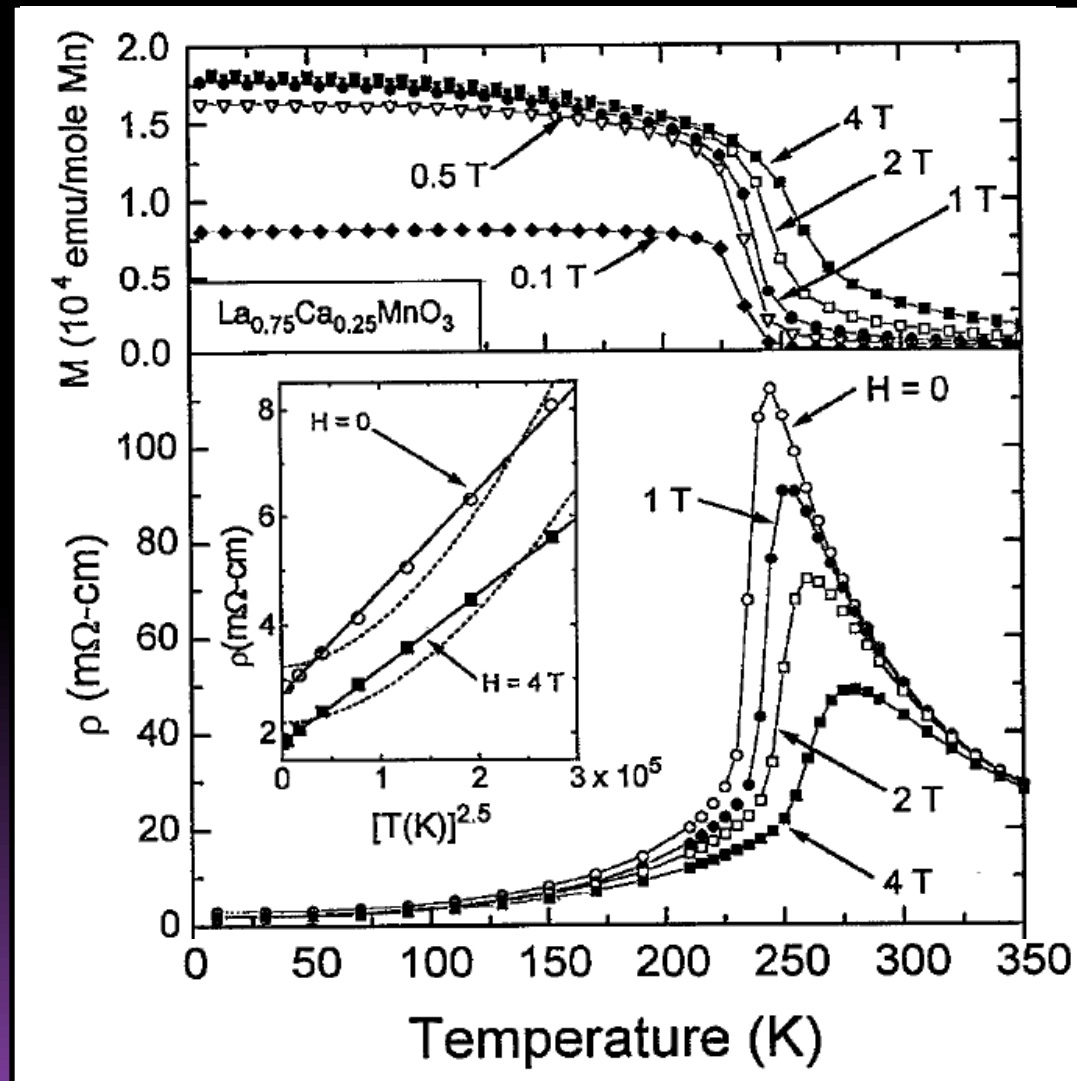
SPAIN



Manganites are well known for

Colossal magnetoresistance

$$MR = \frac{R(H) - R(0)}{R(H)} \times 100\%$$



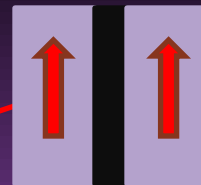
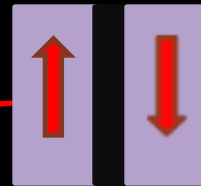
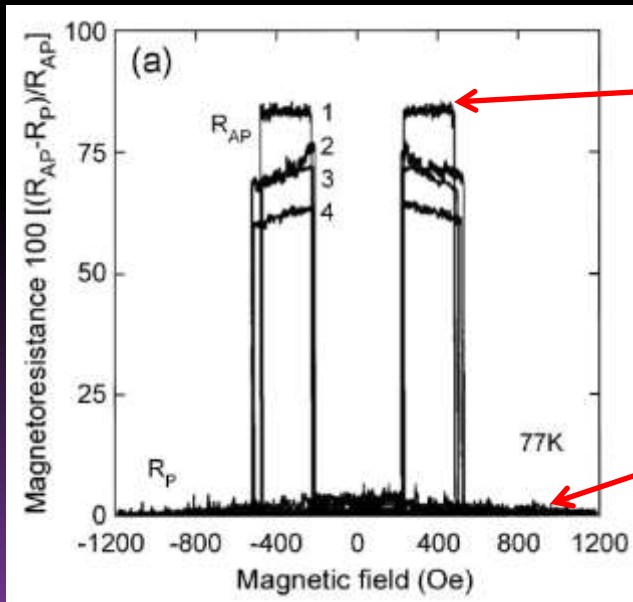
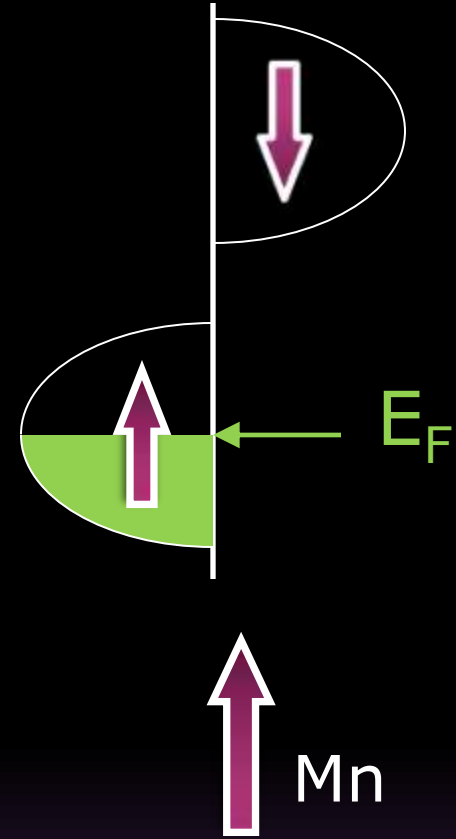
Manganites are well known for

Colossal magnetoresistance

$$MR = \frac{R(H) - R(0)}{R(H)} \times 100\%$$

Half-metals \longrightarrow spintronics

Bibes, Barthélémy, IEEE Trans. Elect. Devices 54, 1003 (2007)



M. Jo et al, PRB 61, R14905 (2000)

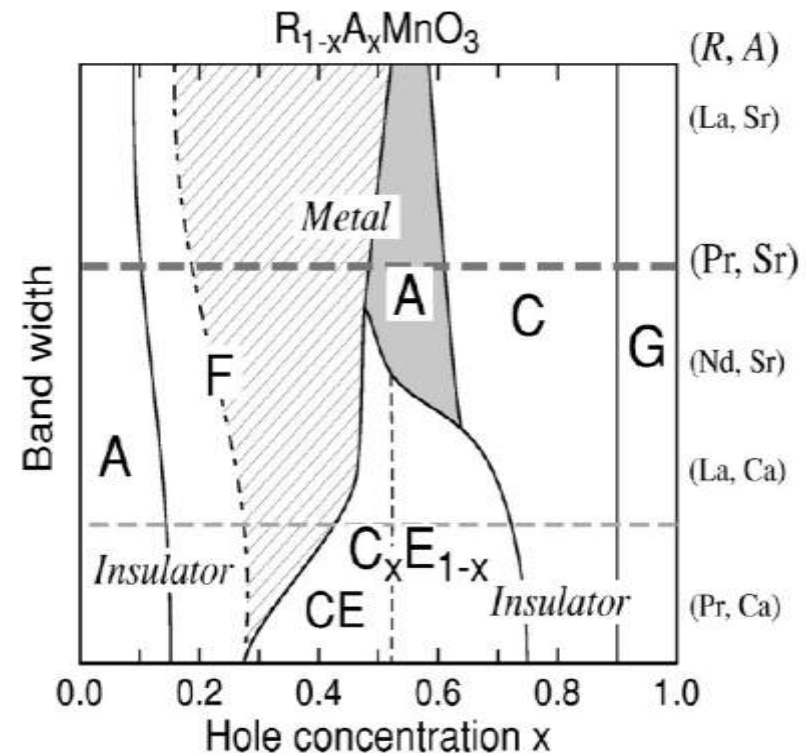
Manganites are well known for

Colossal magnetoresistance

$$MR = \frac{R(H) - R(0)}{R(H)} \times 100\%$$

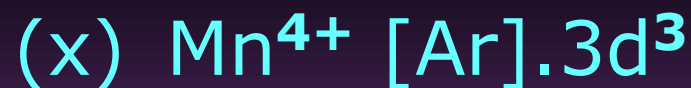
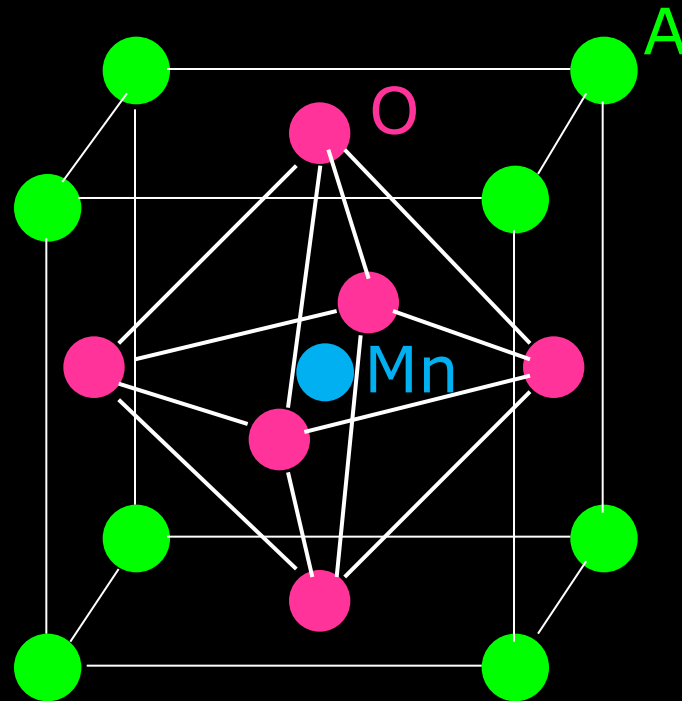
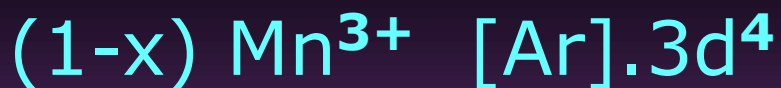
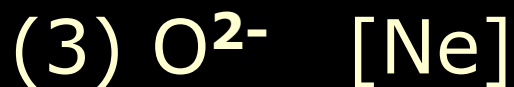
Half-metals \longrightarrow spintronics

Rich phase diagram



Why studying all-manganite heterostructures?

Study competition of very different phases while minimizing lattice effects and keeping chemical similarity



4-x electrons on the Mn d orbitals (mixed valency)

Mn d orbitals

Mn³⁺

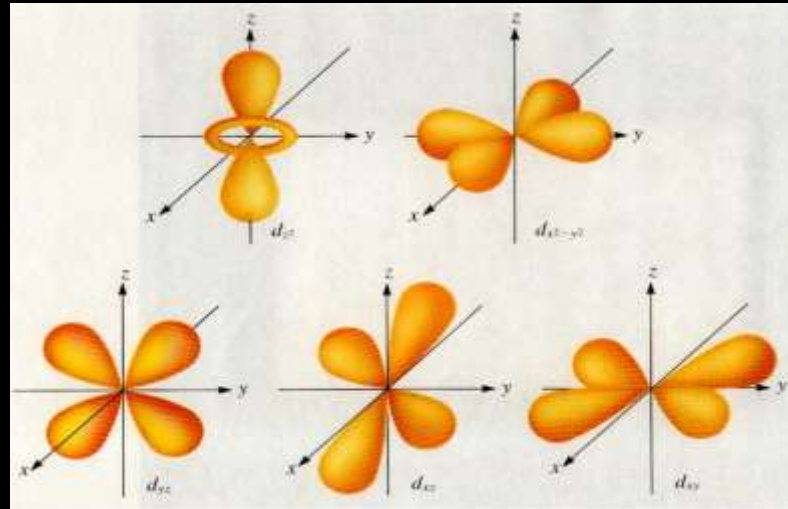
[Ar].3d⁴

Mn⁴⁺

[Ar].3d³

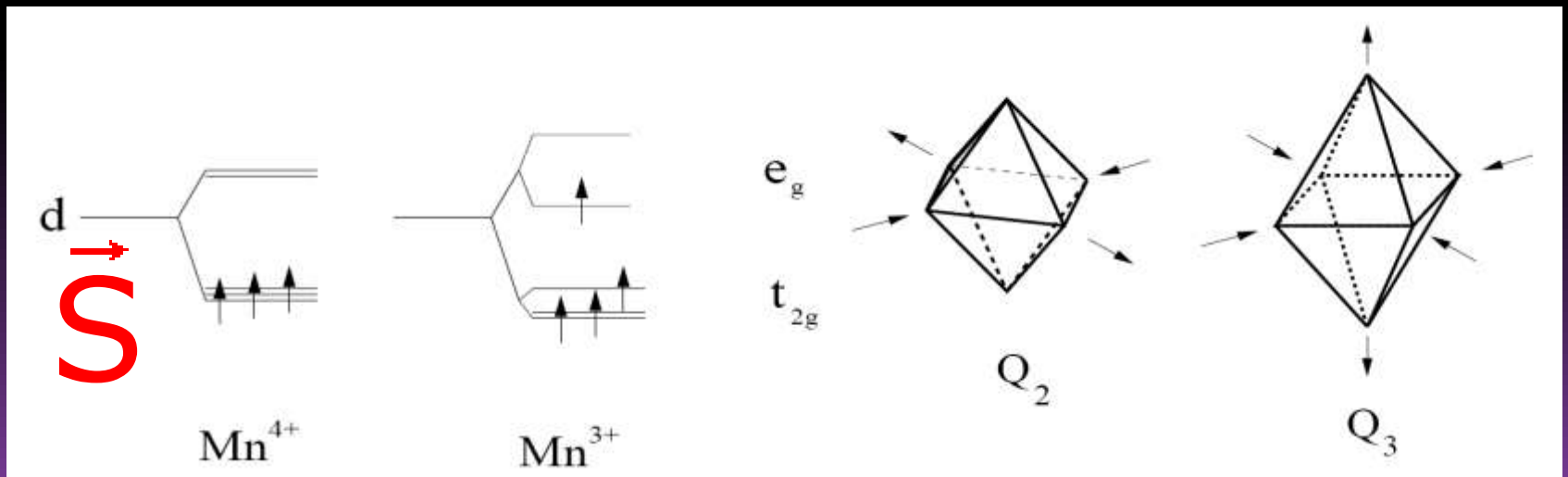
Orbital splittings:

1. Crystal field : splitting of e_g and t_{2g}
2. Jahn-Teller distortions of the octahedra: splitting of the e_g levels



e_g

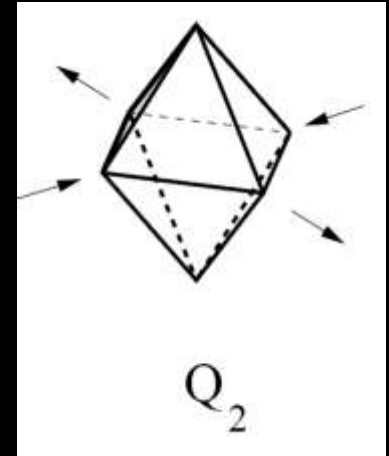
t_{2g}



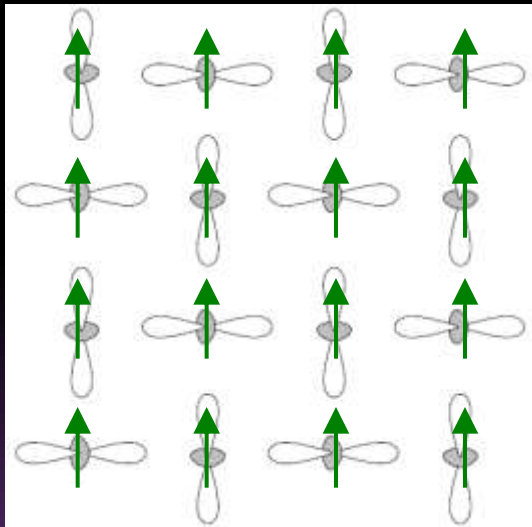
Jahn-Teller distortions are cooperative



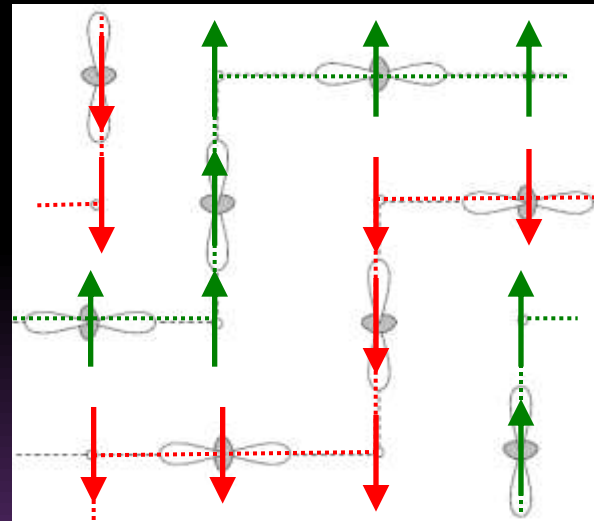
Orbital ordering



$x=0$



$x=0.5$



Orbital order \leftrightarrow magnetic order
(t_{2g} - t_{2g} superexchange is AF)



Competing interactions on manganites

Electron-lattice
Coulomb
AF superexchange

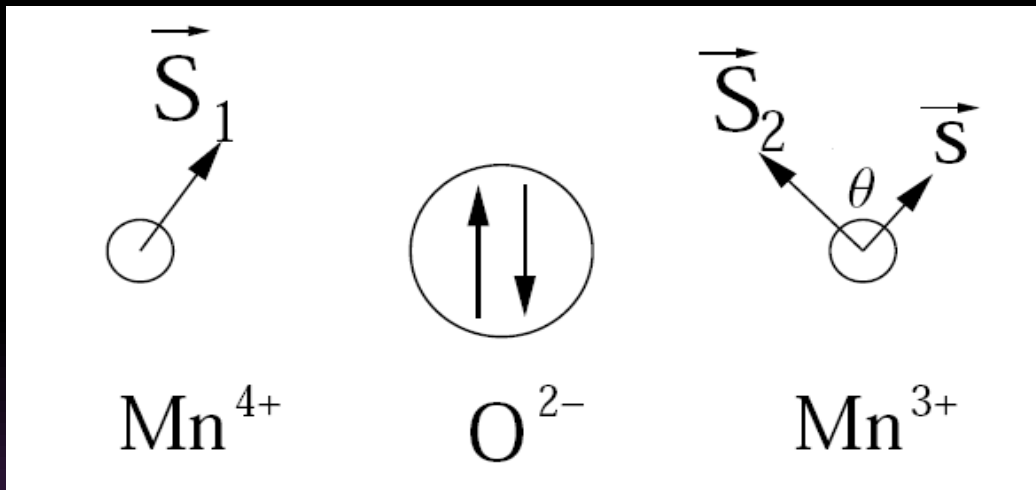


Favour AF and
insulating

Double exchange

Double exchange

$$\sum_{\alpha,\beta} t^{\alpha\beta} \sum_{i,j,\sigma} c_{i,\alpha,\sigma}^\dagger c_{j,\beta,\sigma} + J_H \sum_i S_i s_i \xrightarrow{J_H \rightarrow \infty} \sum_{i,j} \sum_{\alpha,\beta} t_{ij}^{\alpha\beta} d_{i\alpha}^\dagger d_{j\beta}$$



$$t_{ij}^{\alpha\beta} = t^{\alpha\beta} \cos\left(\frac{\theta_{ij}}{2}\right)$$

Favours FM and metal

C. Zener, Phys. Rev. **82**, 403, (1951)

P. W. Anderson y A. Hasegawa, Phys Rev **100**, 675 (1955)

Competing interactions on manganites

Electron-lattice
Coulomb
AF superexchange



Favour AF and
insulating

Double exchange



Favours FM and
metal



All-manganite heterostructures

SrMnO_3 / LaMnO_3
(AF band insulator / AF Mott insulator)



metallic (similar to $\text{SrTiO}_3/\text{LaTiO}_3$)
and ferromagnetic (double exchange)

Experiments:

Koida et al, PRB 66, 144418 (2002)

S. Smadici et al, PRL 99, 196404 (2007)

May et al, Physical Review B 77, 174409 (2008)

Theory:

Lin et al, PRB 73, 041104(R) (2006); ibid 78, 184405 (2008)

Nanda, Satpathy Phys. Rev. Lett. 101, 127201 (2008)

Outline

1. Description of the model

2. An all-manganite insulator/insulator heterostructure
(with J. Salafranca and L. Brey)

3. Metal/insulator heterostructure: an AF insulating
manganite turning into a spin-filter
(with Z. Sefrioui, C. Visani, K. March, C. Carrétéro,
M. Walls, A. Rivera-Calzada, C. León, R. López Antón,
T.R. Charlton, F.A. Cuéllar, E. Iborra, F. Ott, D. Imhoff,
L. Brey, M. Bibes, J. Santamaría *and* A. Barthélémy)

Model

Double-exchange + electron-lattice + AF superexchange + Coulomb

Double exchange $\sum_{i,j} \sum_{\alpha,\beta} t^{\alpha\beta} \cos\left(\frac{\theta_{ij}}{2}\right) d_{i\alpha}^\dagger d_{j\beta}$

Electron-lattice $\sum_i \beta Q_{1i}^2 + Q_{2i}^2 + Q_{3i}^2 - \lambda(Q_{1i}\rho_i + Q_{2i}\tau_i^x + Q_{3i}\tau_i^z)$

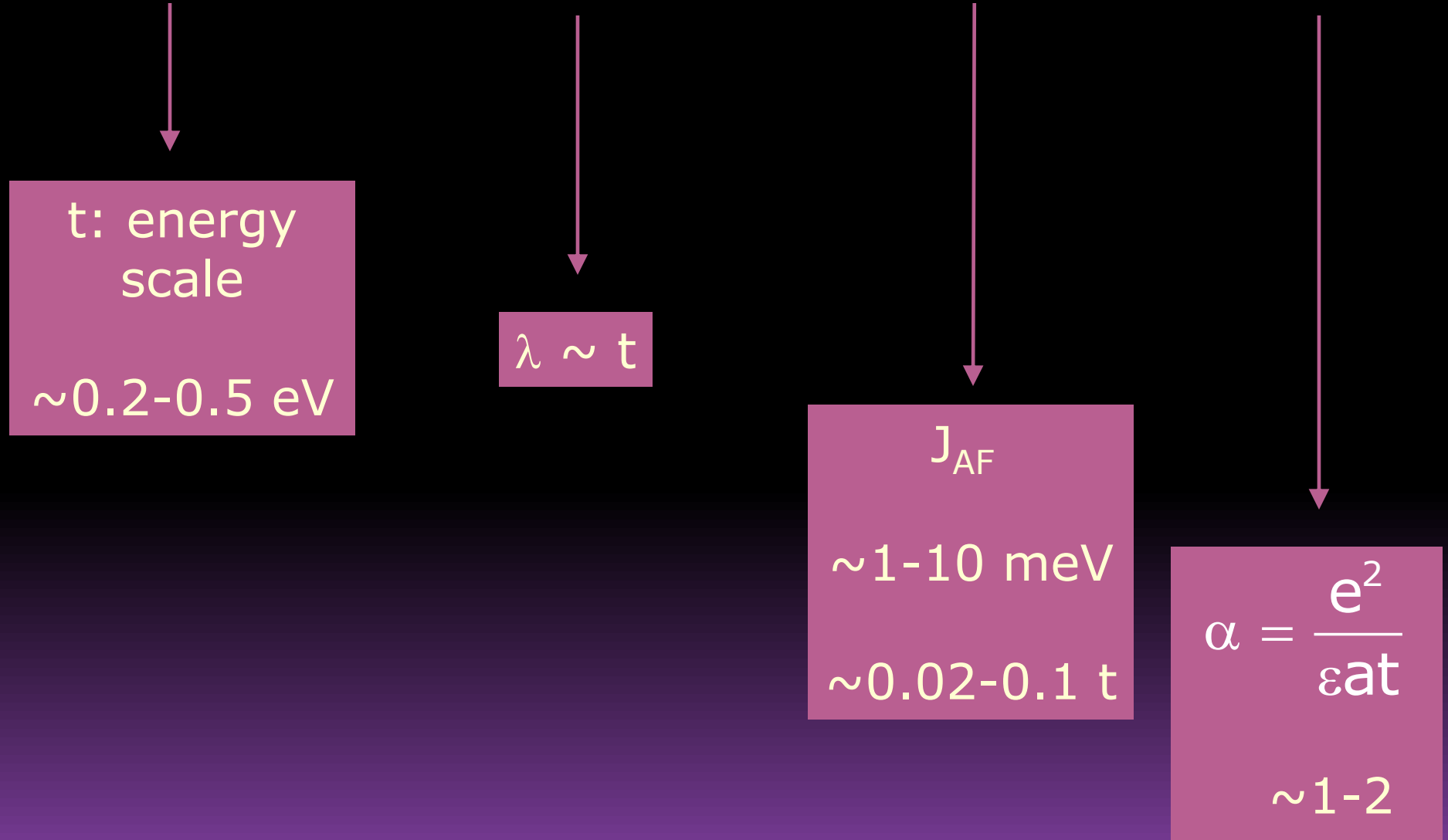
AF SE between the t_{2g} electrons $J_{AF} \sum_{ij} \mathbf{S}_i \mathbf{S}_j$

Long range Coulomb interaction: Hartree

$$\frac{e^2}{\epsilon} \sum_{i \neq j} \left(\frac{1}{2} \frac{\langle n_i \rangle \langle n_j \rangle}{|\mathbf{R}_i - \mathbf{R}_j|} + \frac{1}{2} \frac{Z_i Z_j}{|\mathbf{R}_i^A - \mathbf{R}_j^A|} - \frac{Z_i \langle n_j \rangle}{|\mathbf{R}_i^A - \mathbf{R}_j|} \right)$$

Model

Double-exchange + electron-lattice + AF superexchange + Coulomb



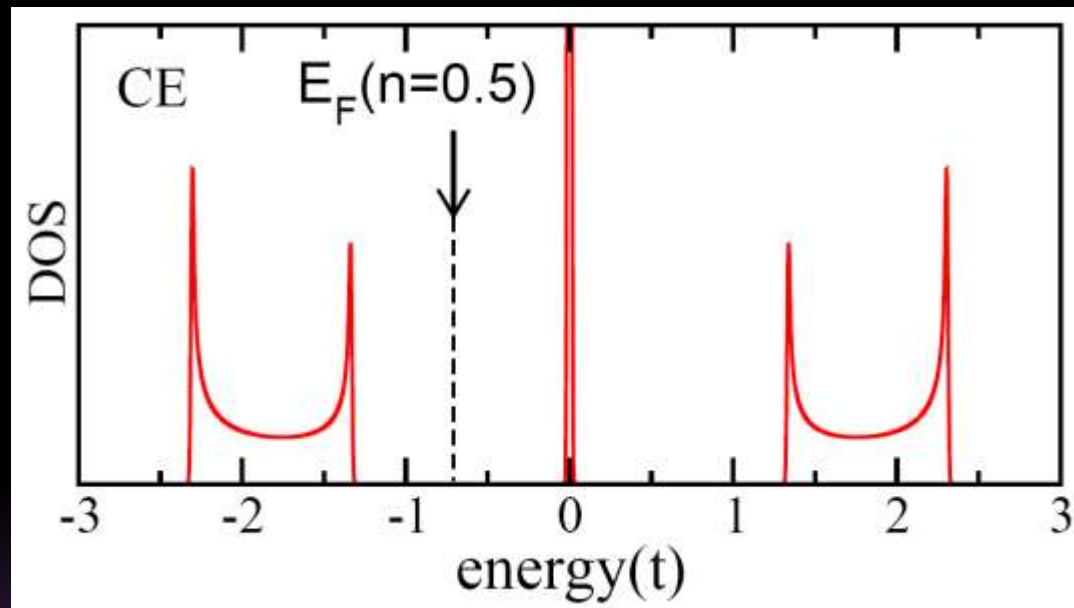
2 AF insulators: $\text{CaMnO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$

CaMnO_3

$\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$

CaMnO_3

$\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$: AF and charge/orbital ordered insulator



$n > 0.5$ adding electrons very costly \rightarrow phase separation (CE/FM)

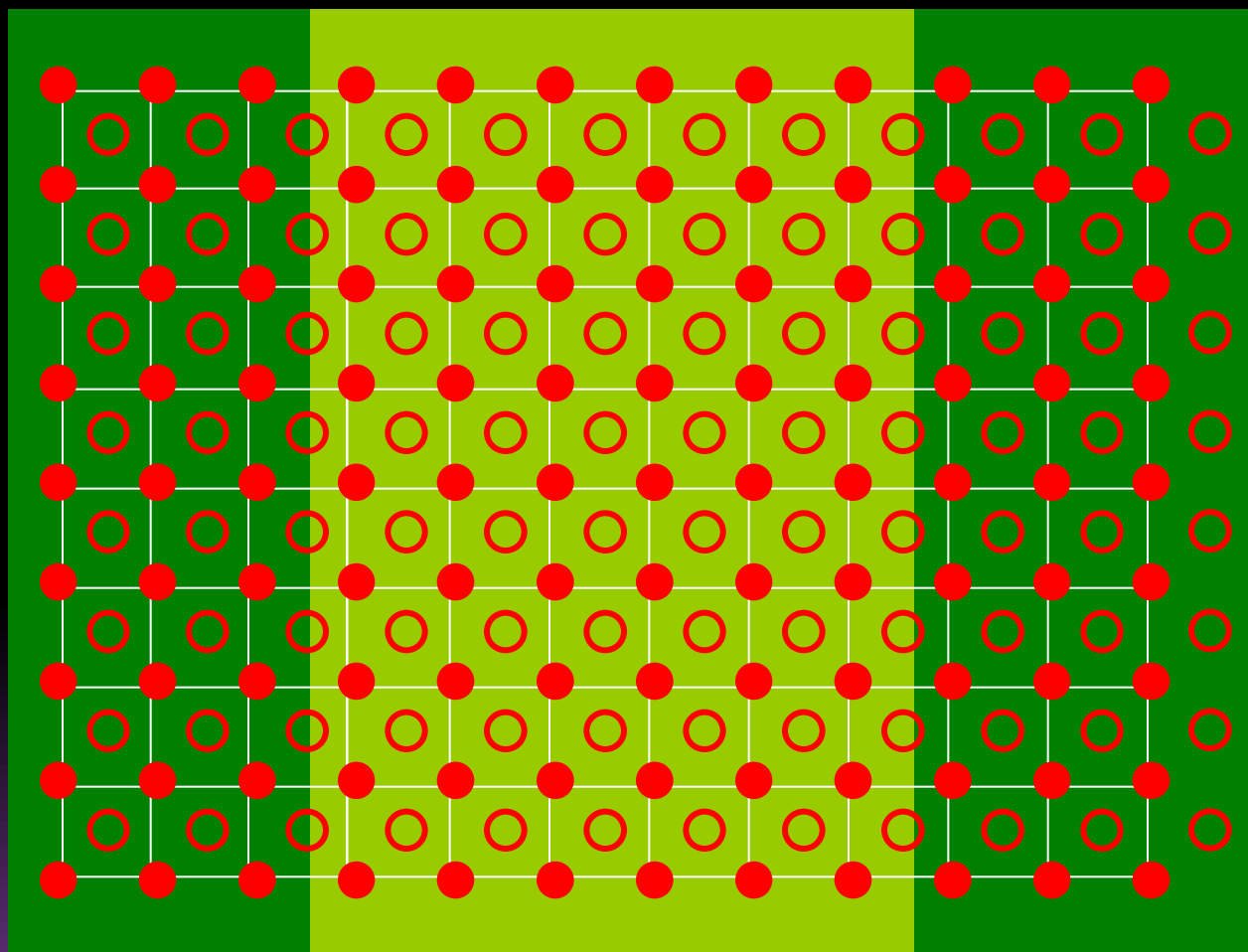
$n < 0.5$ in principle, removing electrons not costly
in practice, incommensurate order opens a gap at E_F

2 AF insulators: $\text{CaMnO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$

CaMnO_3

$\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$

CaMnO_3

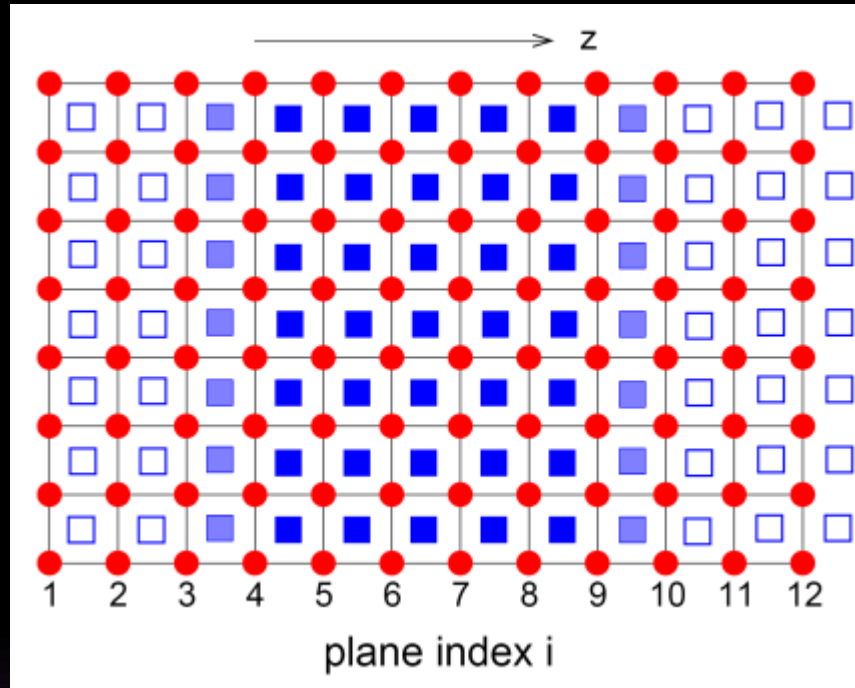


→ z

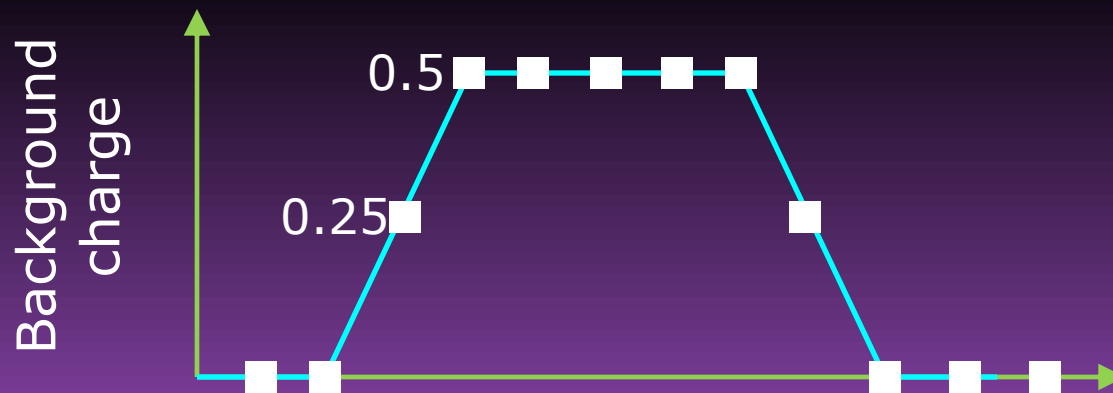
○ La, Ca
● Mn

2 AF insulators: $\text{CaMnO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$

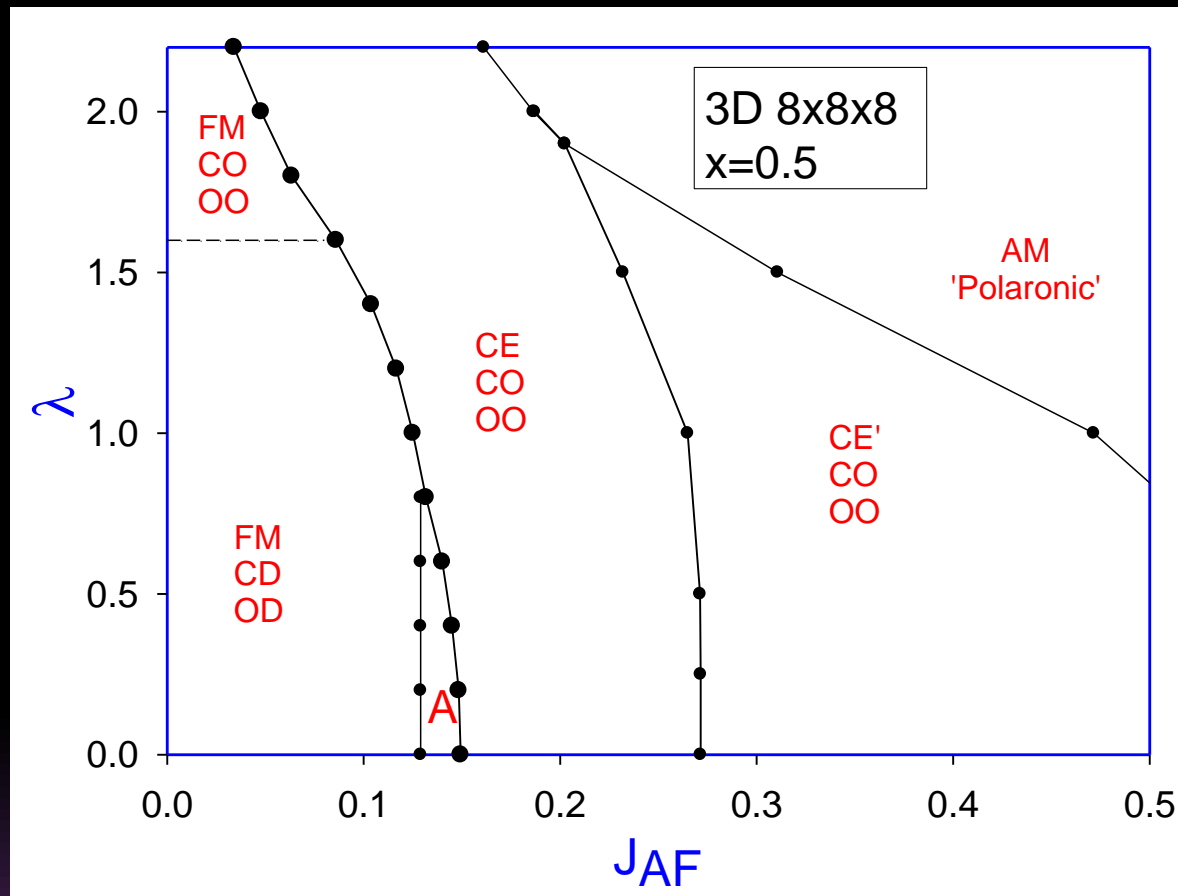
CaMnO_3 $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ CaMnO_3



4 x 4 cross section,
periodic boundary
conditions



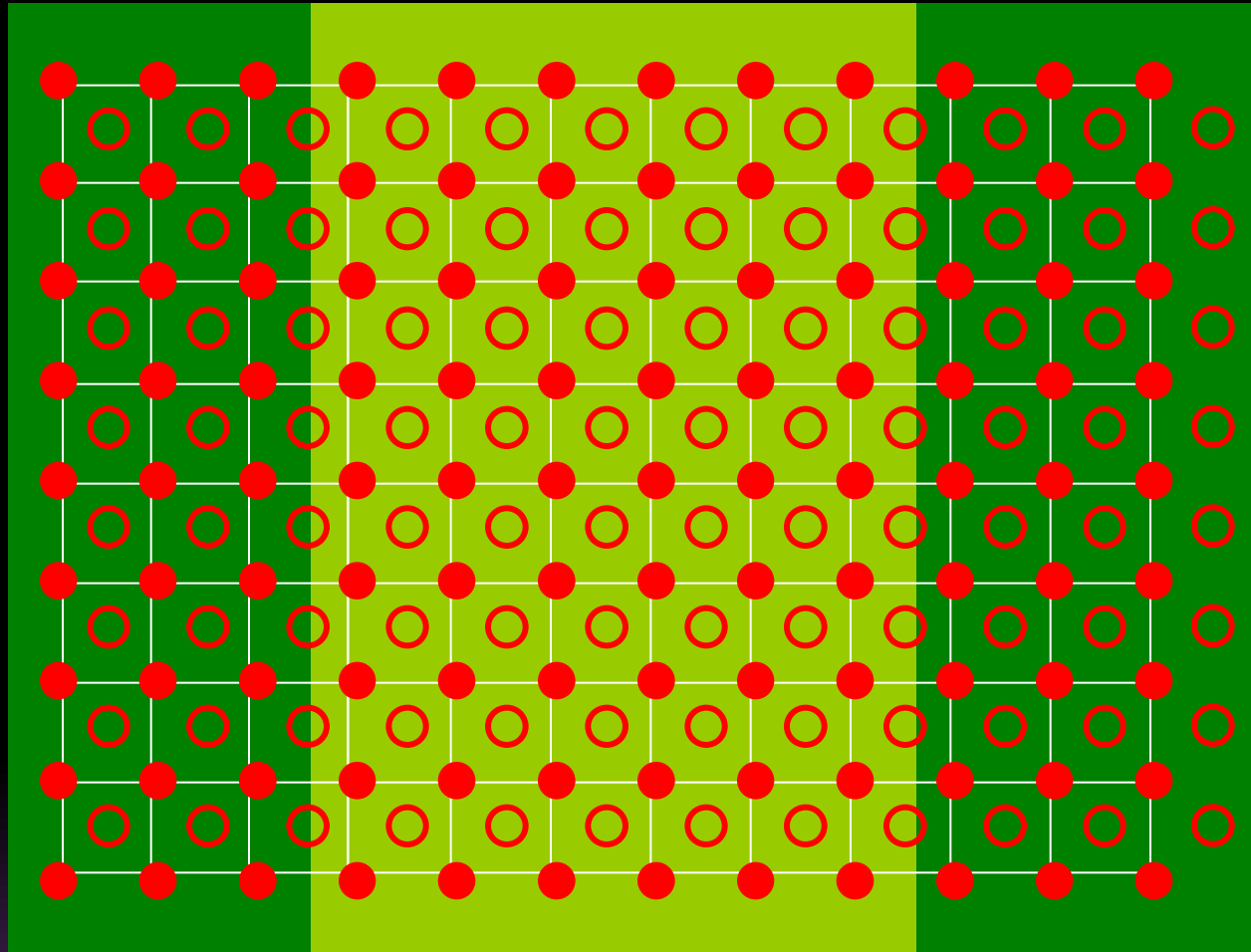
Simplification in the model



L. Brey

$$(\lambda, J_{AF}) \rightarrow J_{AF}^{effec}$$

Phase diagram: OFM



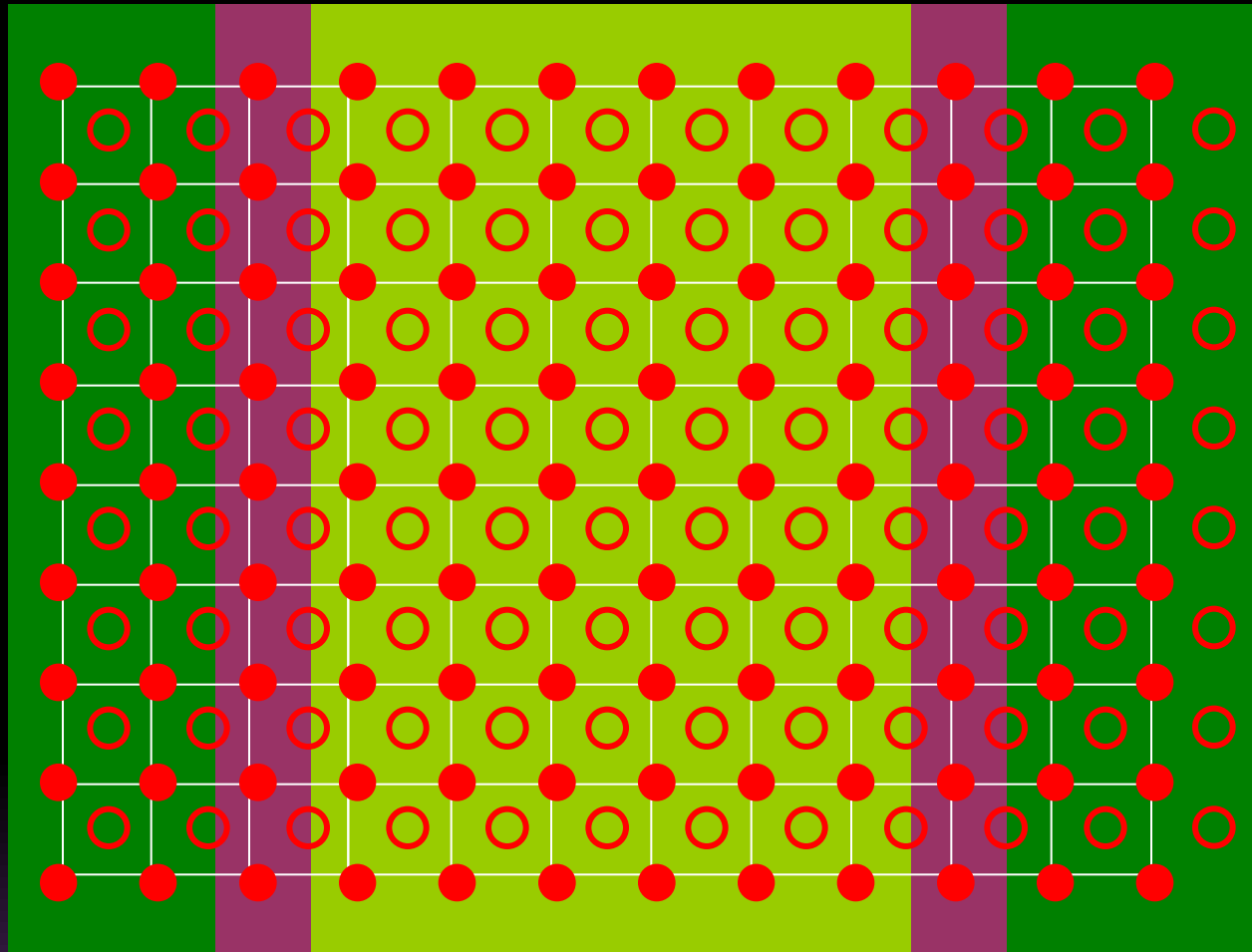
G-AF

CE-AF

G-AF



Phase diagram: 1FM



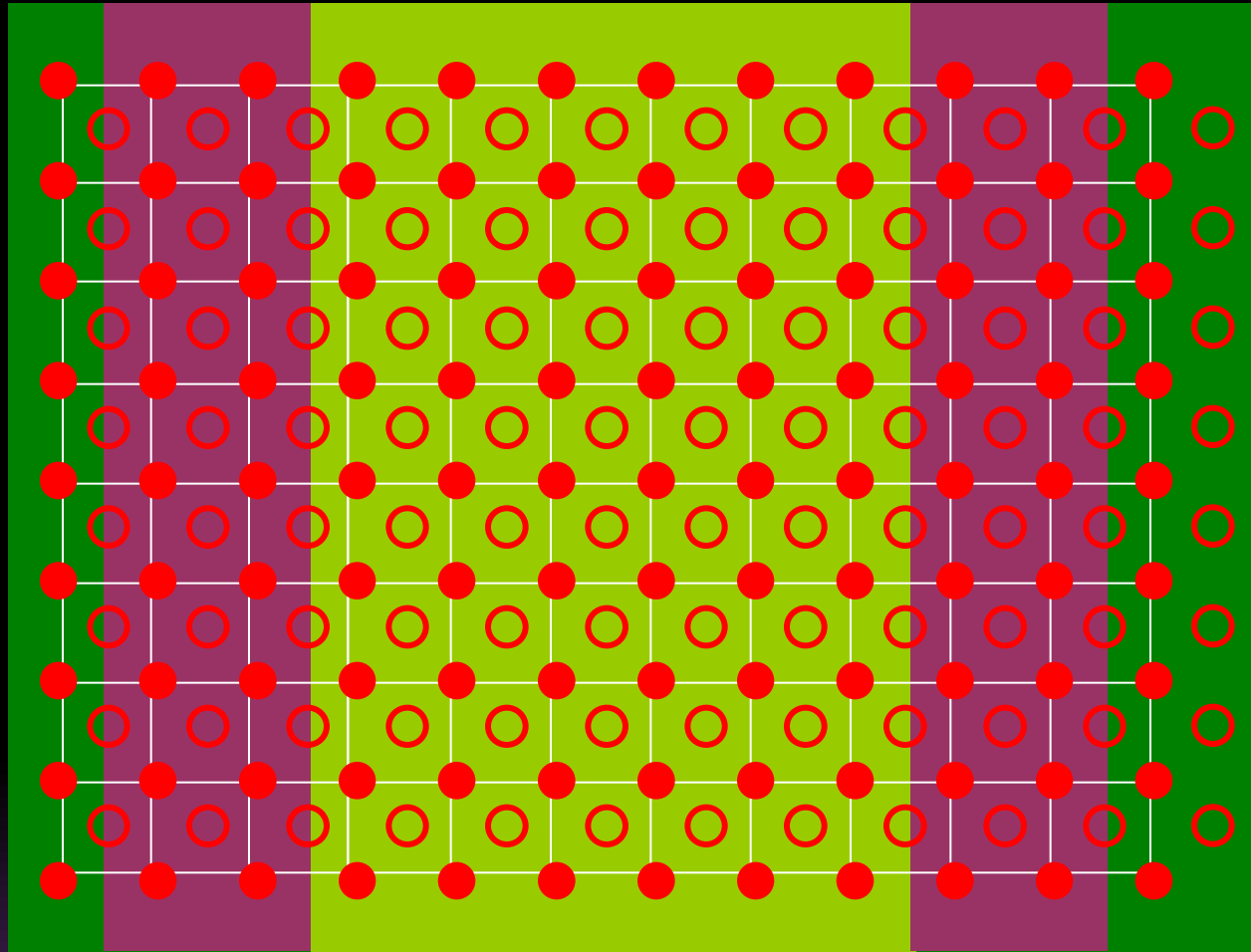
G-AF FM

CE-AF

FM G-AF



Phase diagram: 2FM



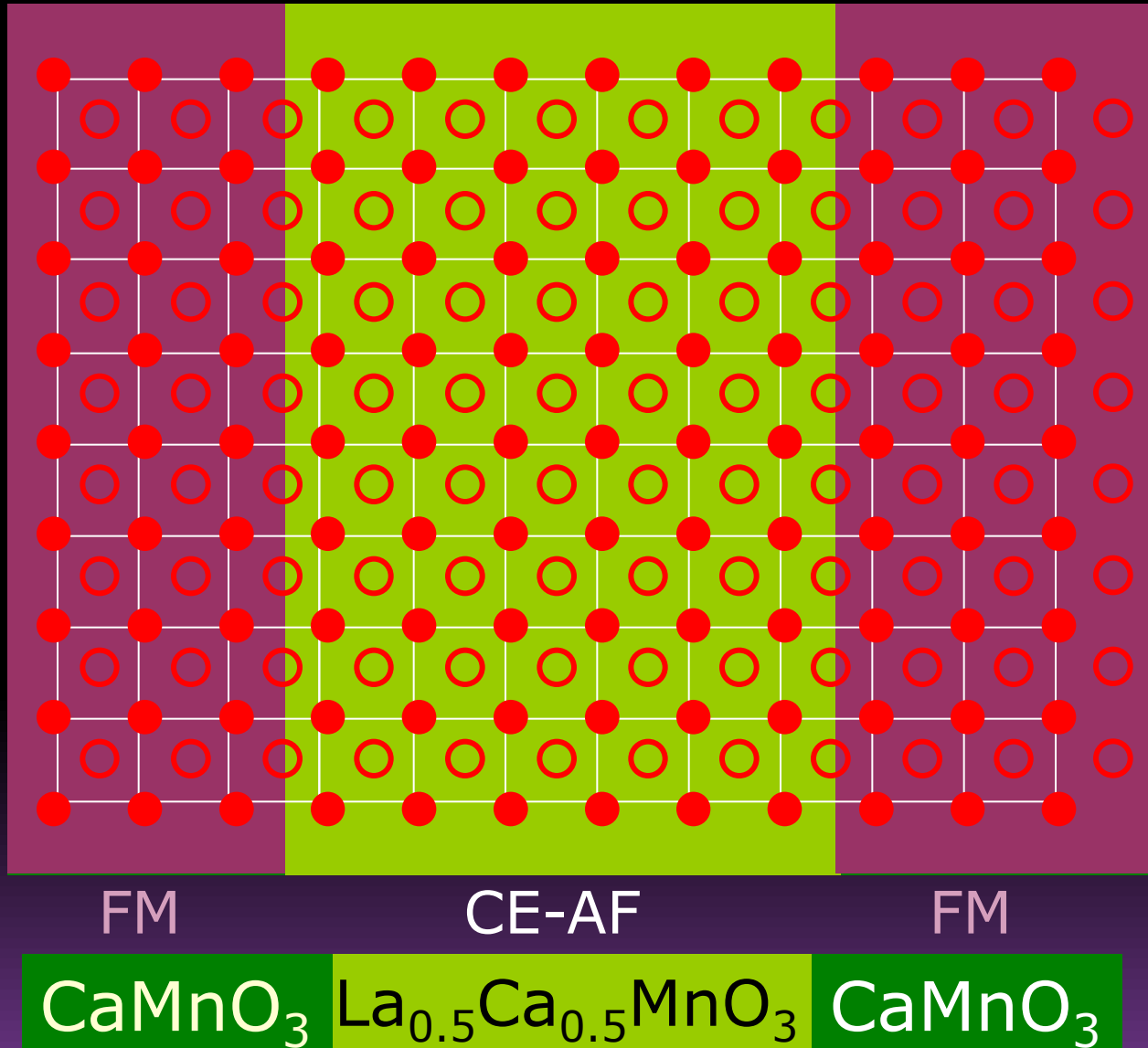
G-AF FM

CE-AF

FM G-AF

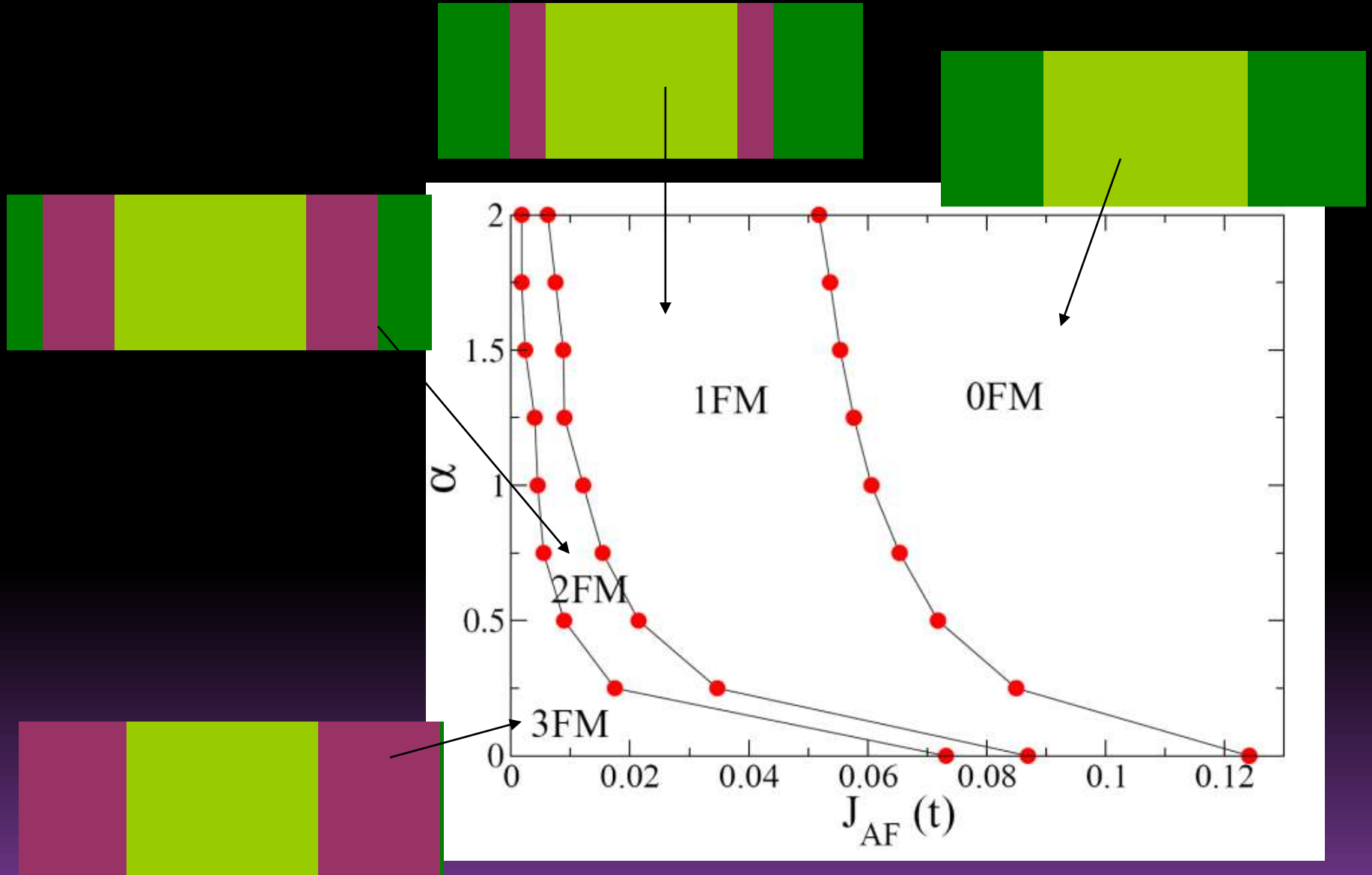


Phase diagram: 3FM

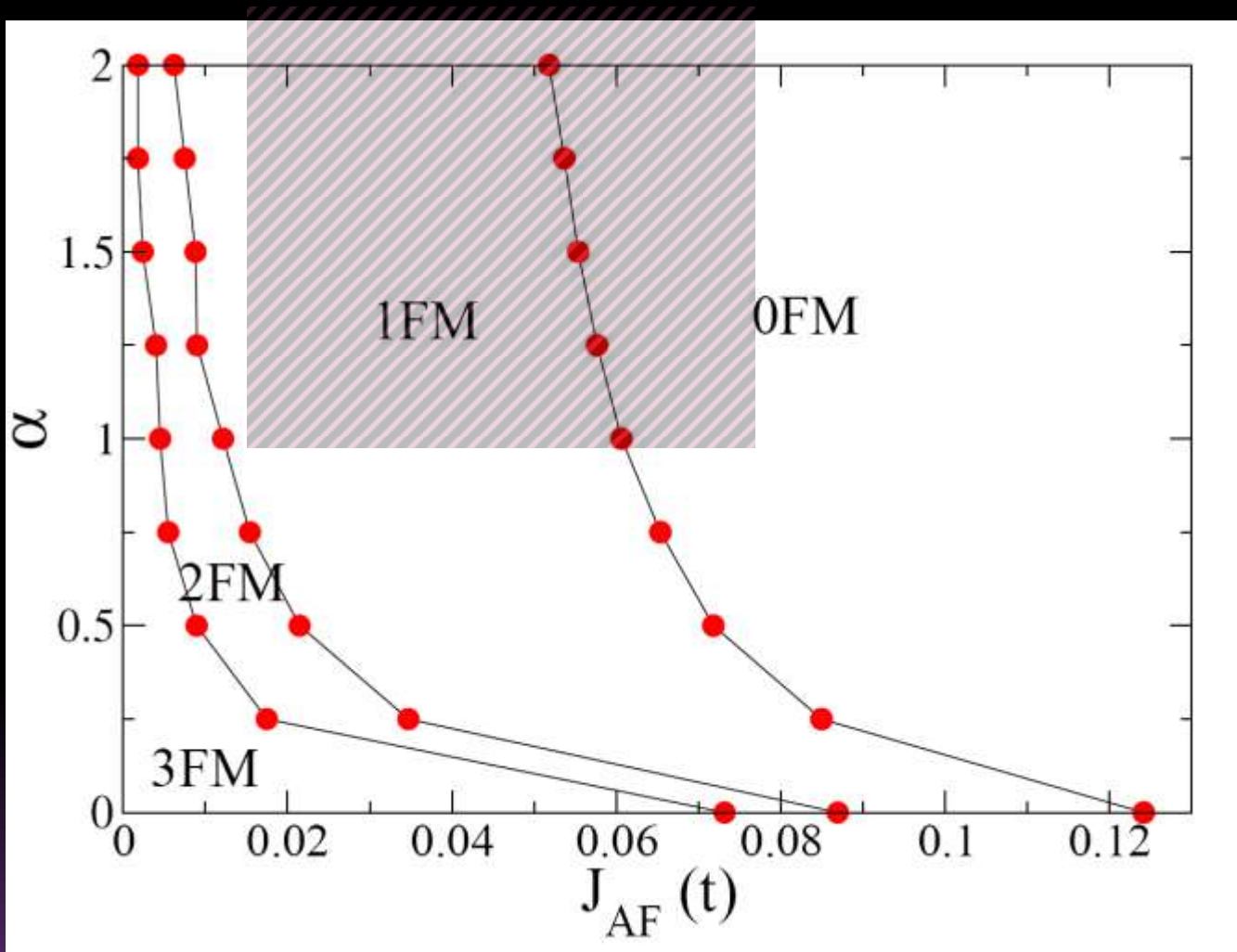


✓ Having FM planes in the CE-AF layer is not favoured

Phase diagram



Phase diagram

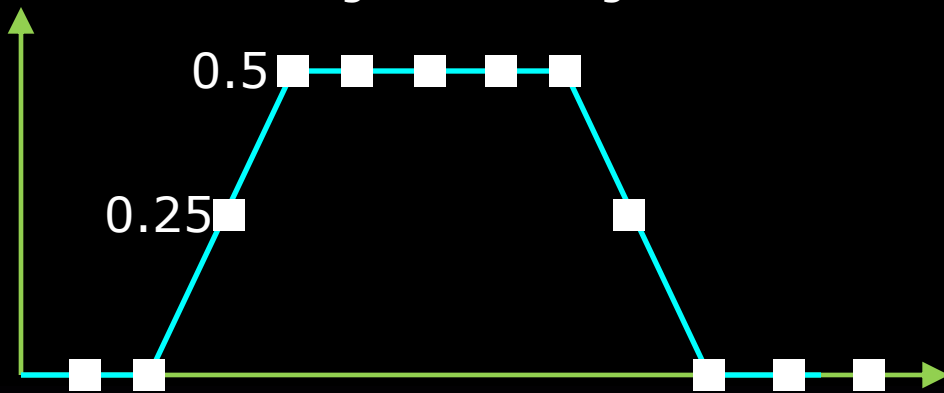


Focus on 1FM configuration

1 FM configuration

Spreading of charge across the interface

Background charge

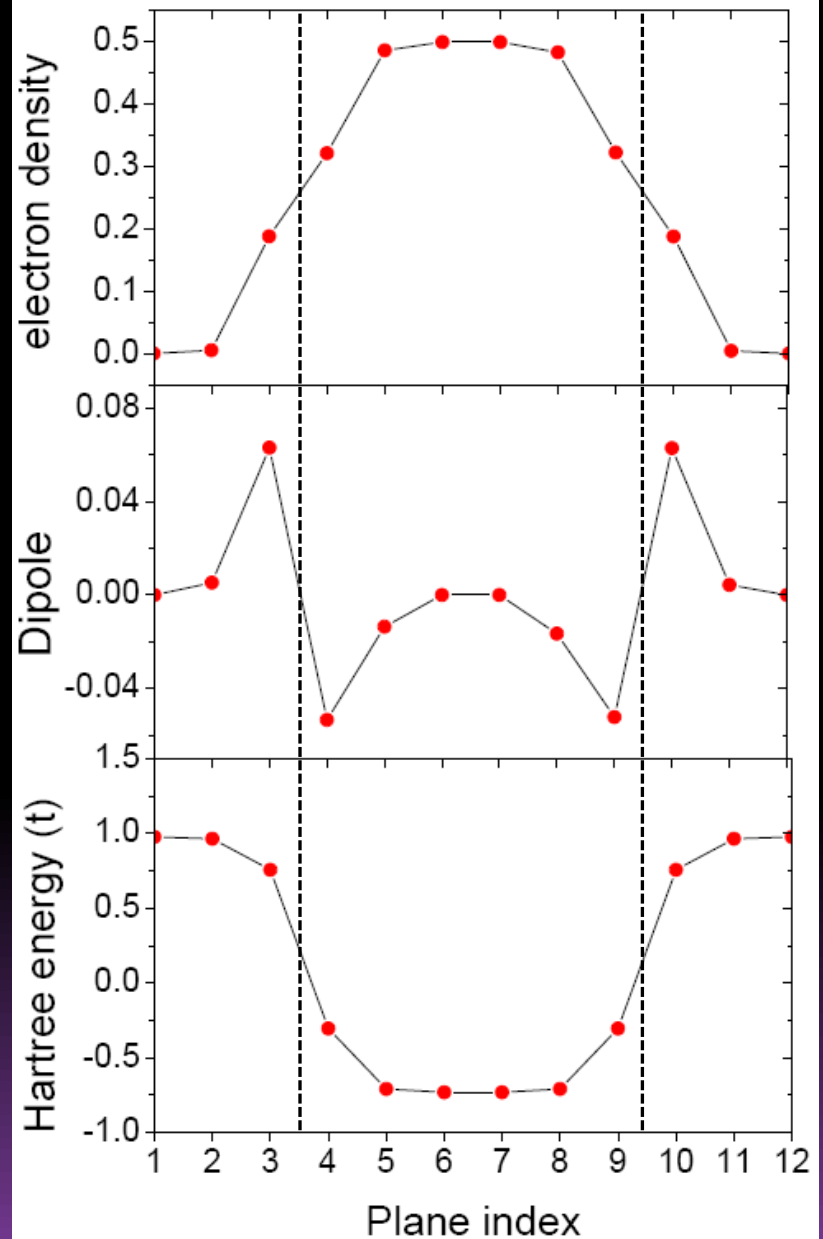


... limited by the Hartree potential

CaMnO₃

La_{0.5}Ca_{0.5}MnO₃

CaMnO₃



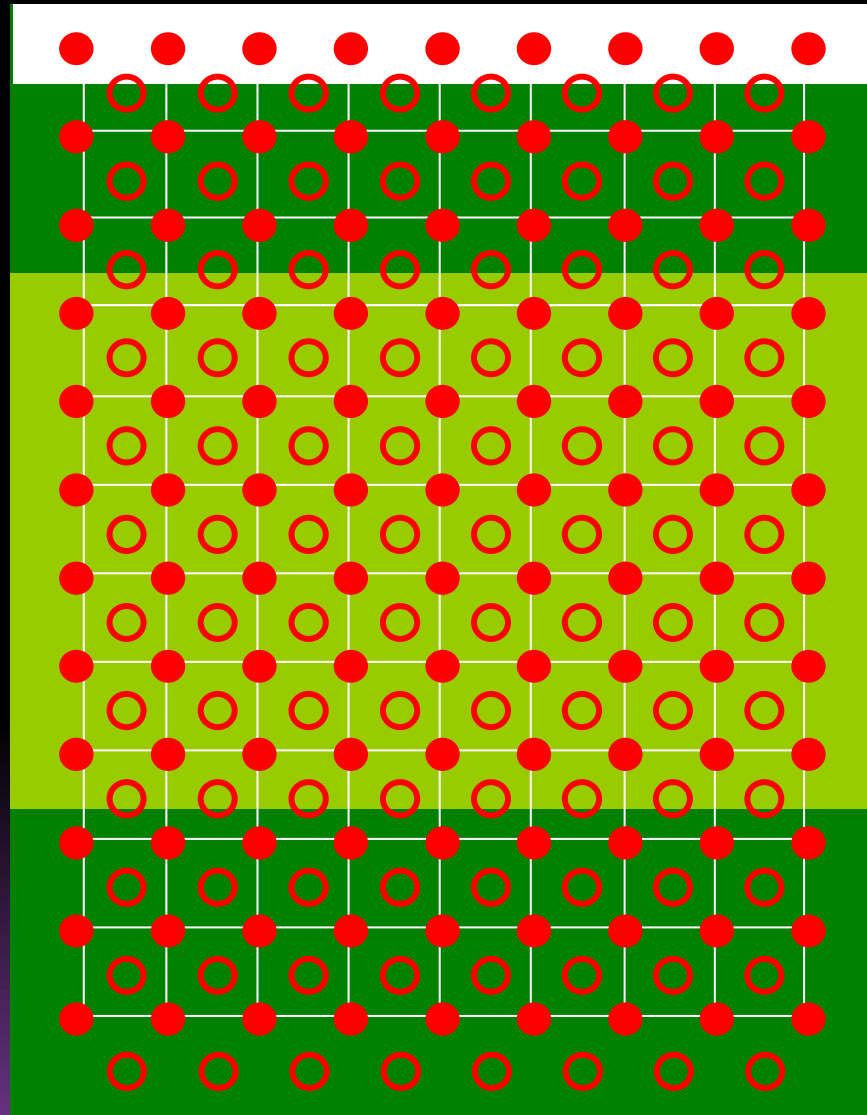
Plane by plane analysis

On each plane we look at:

- ✓ Density of states
- ✓ Charge distribution
- ✓ In-plane conductance

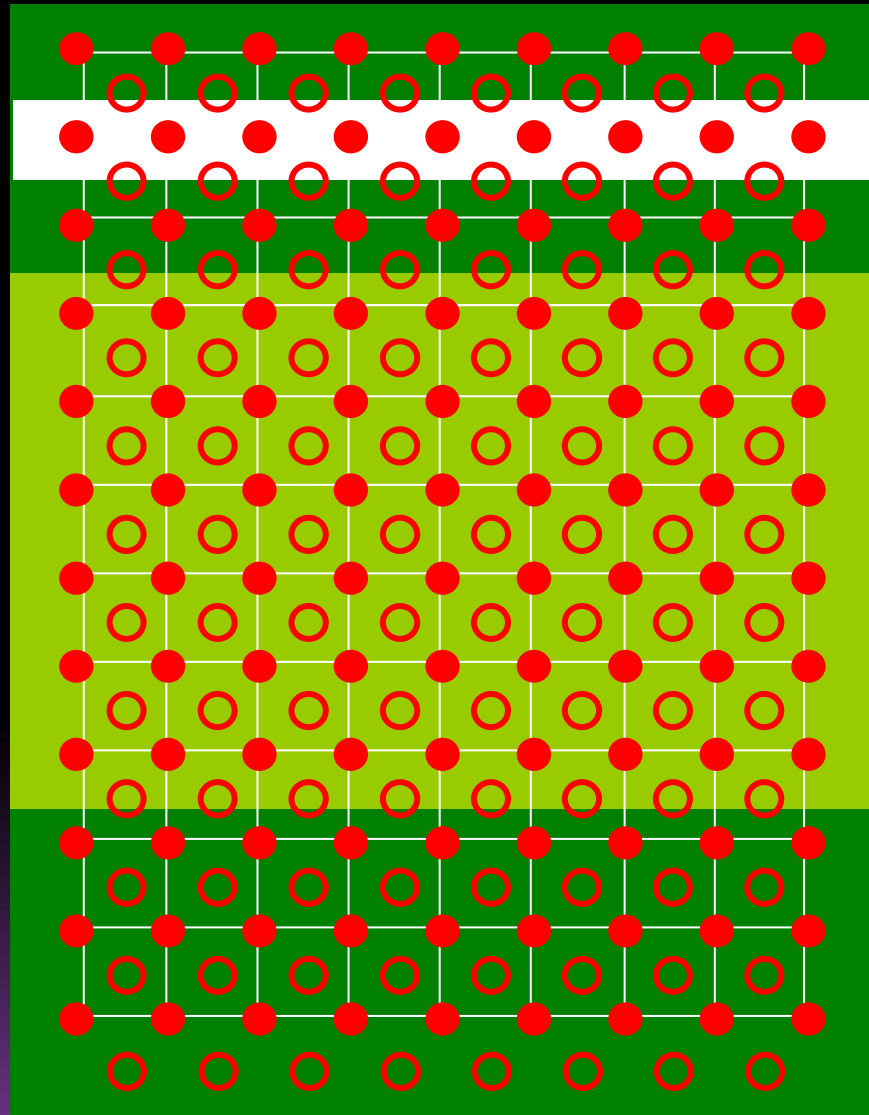
Plane by plane analysis

$i=1$



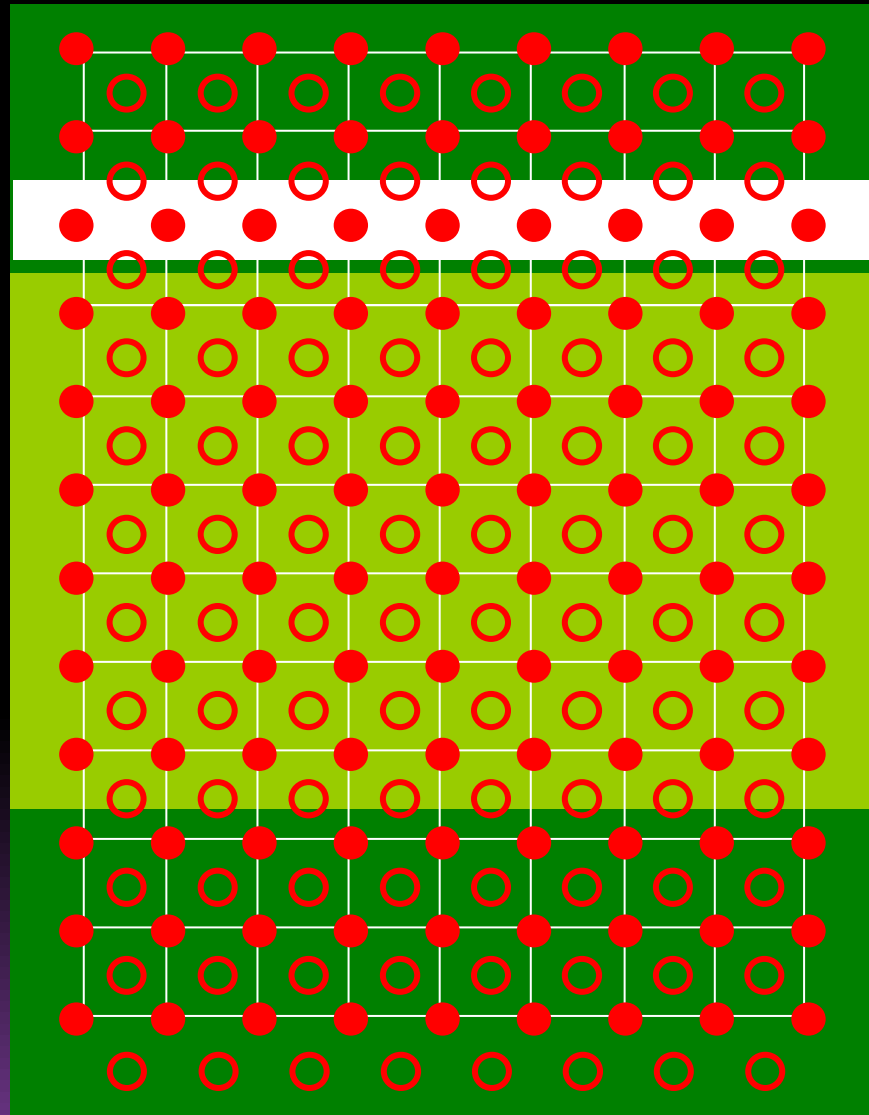
Plane by plane analysis

$i=2$

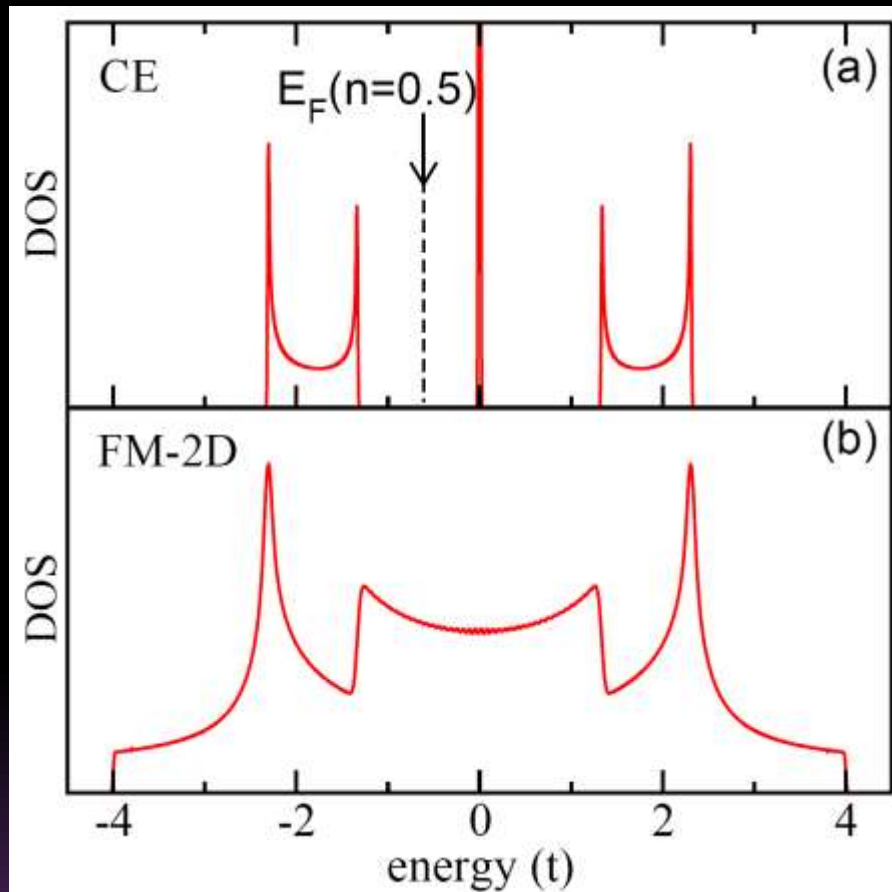


Plane by plane analysis

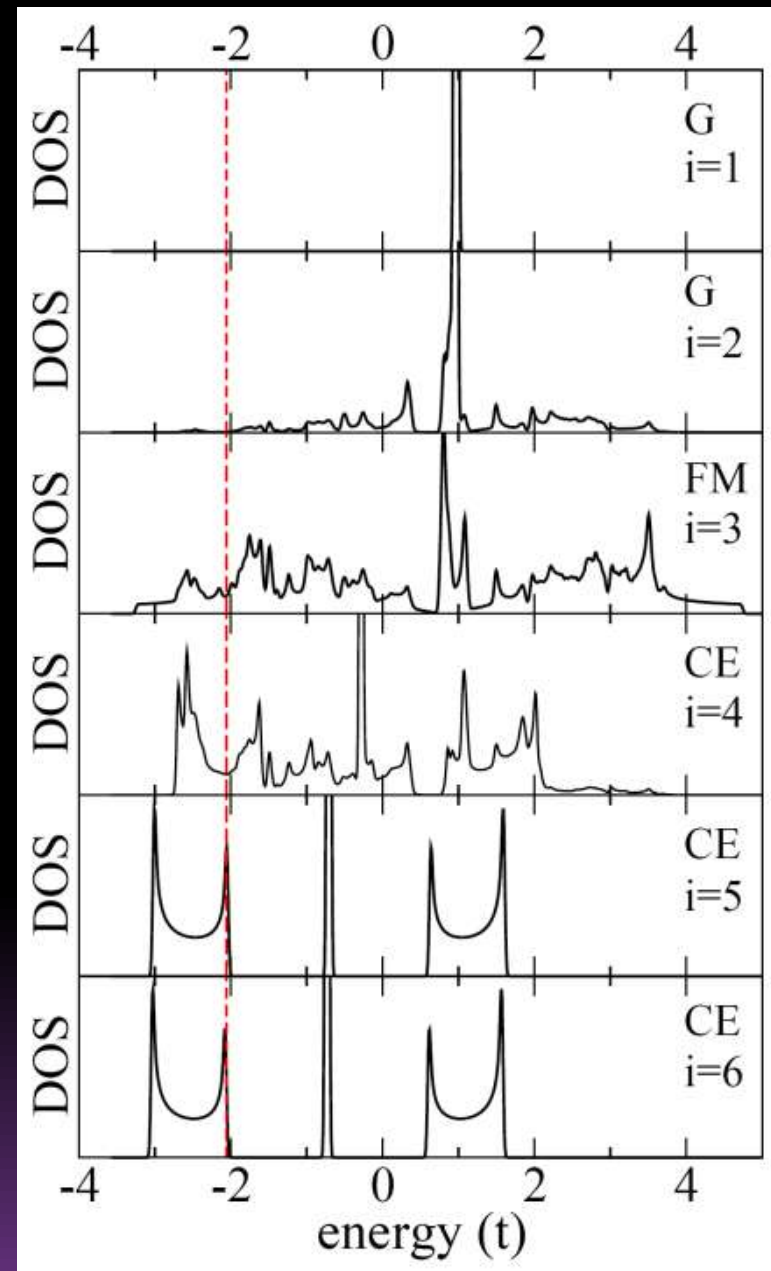
$i=3$



DOS on each plane



Isolated 2D planes

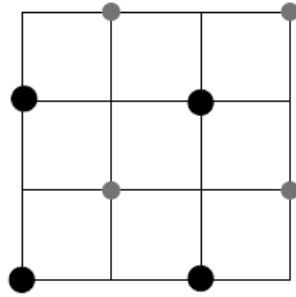
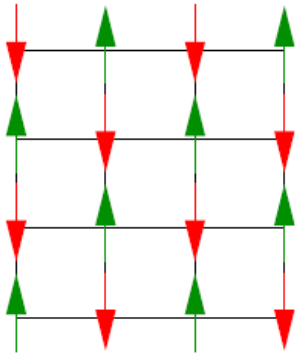


In the heterostructure

Charge/orbital distribution: Shadow order

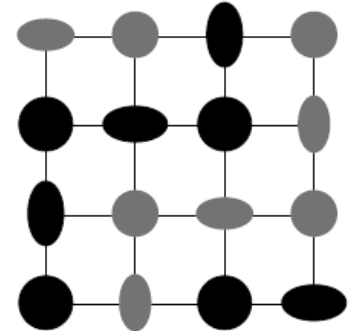
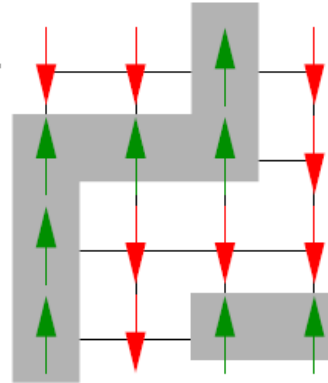
$i=2$

G



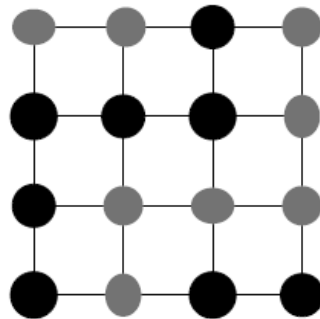
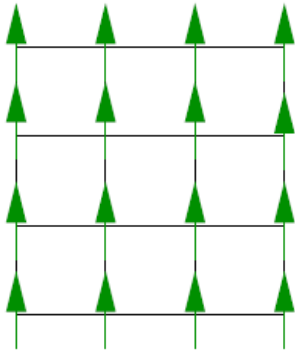
$i=4$

CE



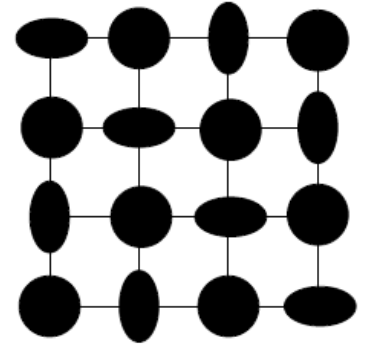
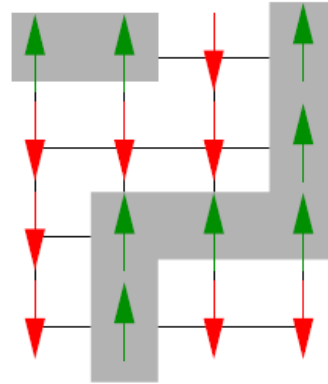
$i=3$

FM

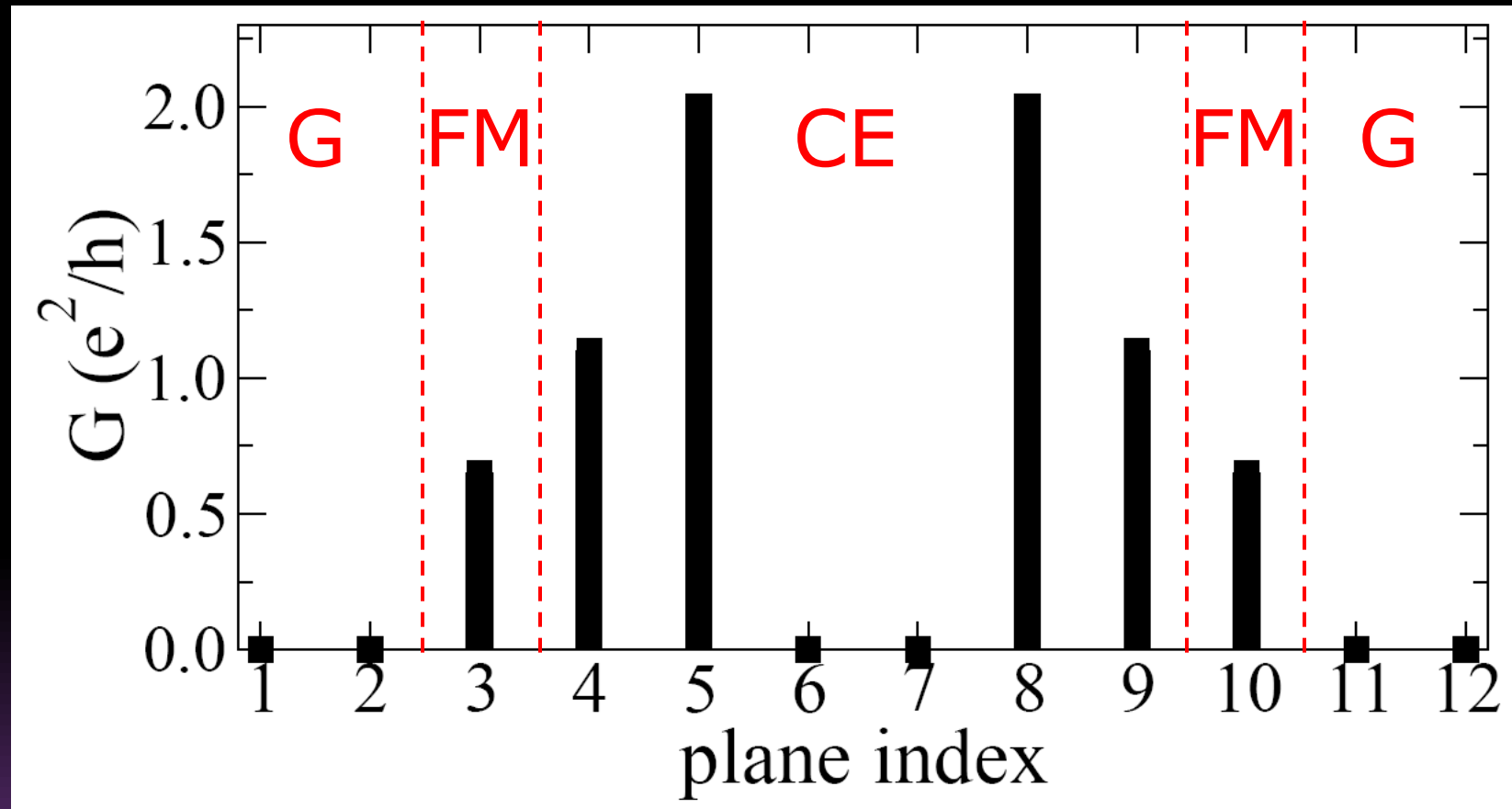


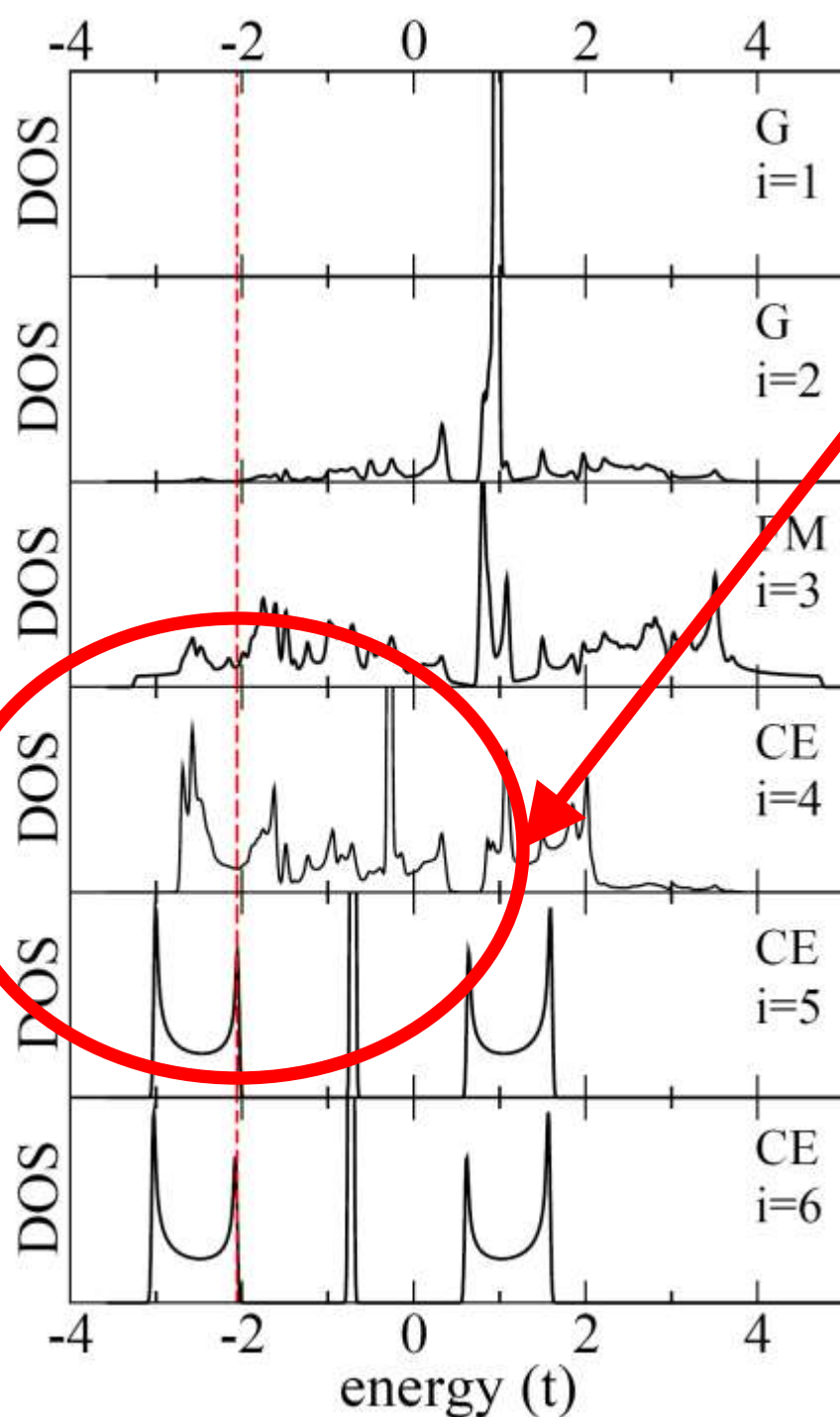
$i=5$

CE



In-plane conductance: Kubo formula

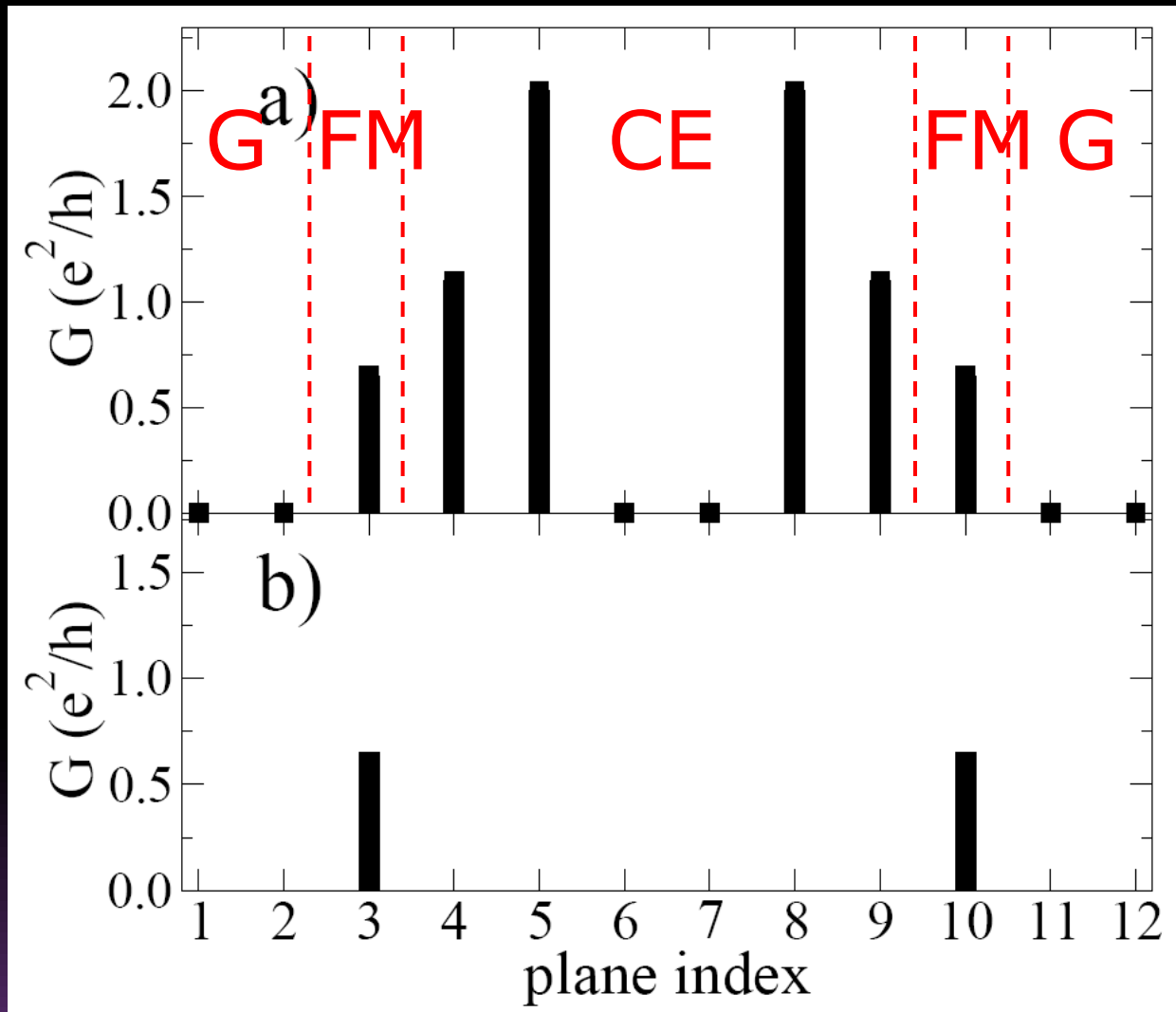




Finite DOS at
Fermi energy
for $i=4, 5!!!$

It is possible that
other complicate
orders (or phase
separation) arose in
planes $i=4, 5$ leading
to insulating behaviour

Conductance on each plane



Only the FM planes are metallic

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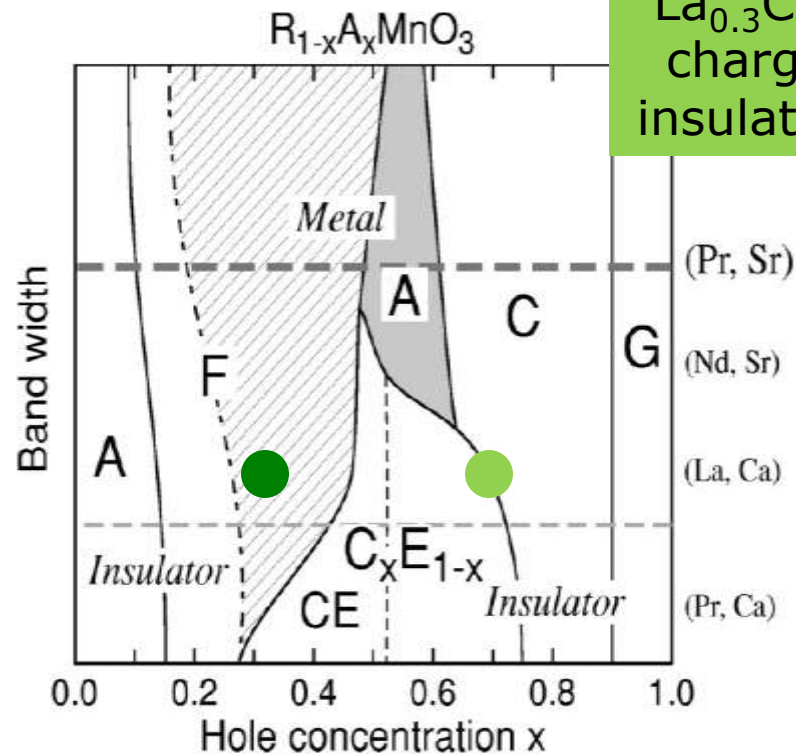
8 nm



1.2 nm: 3 unit cells



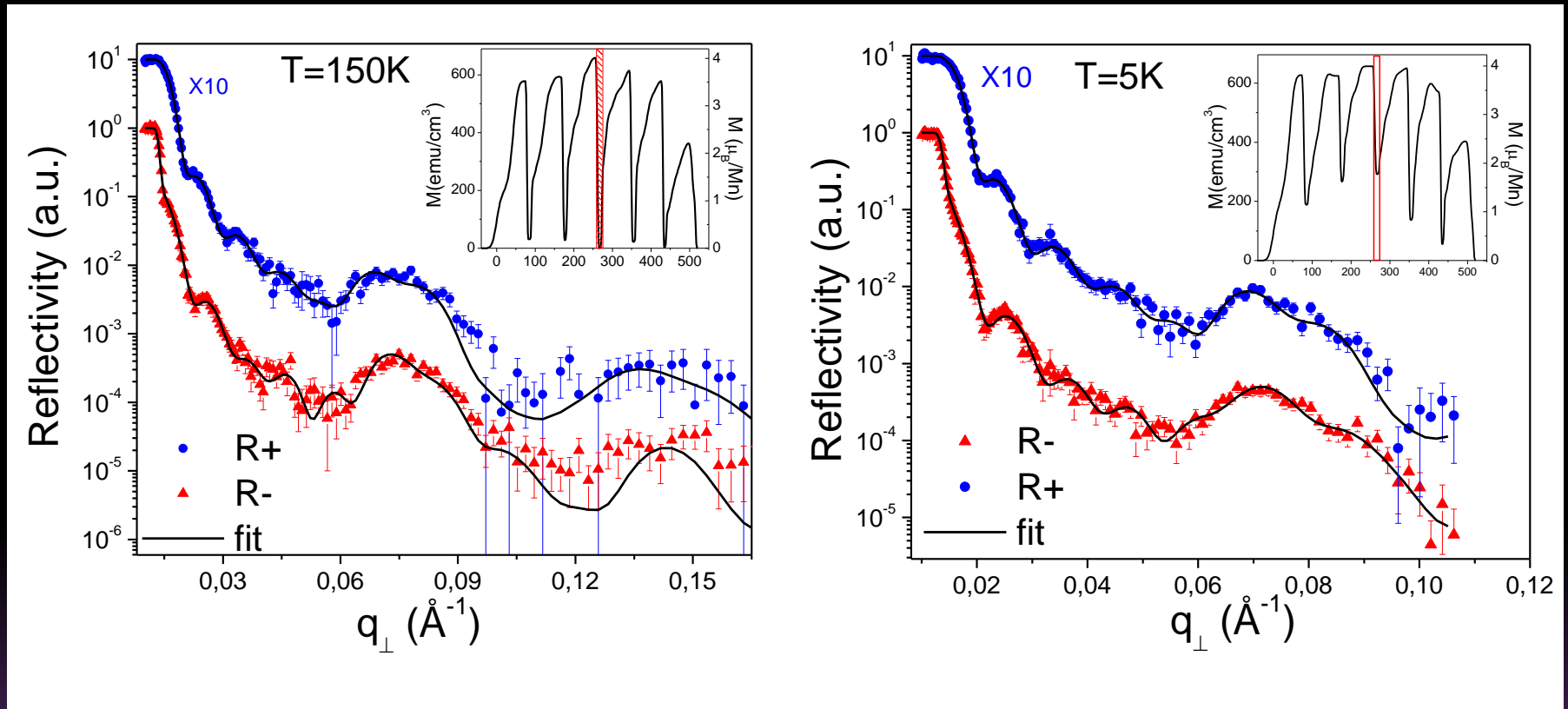
$\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$:
FM half-metal
(electrodes)



$\text{La}_{0.3}\text{Ca}_{0.7}\text{MnO}_3$: AF and
charge/orbital ordered
insulator (tunnel barrier)

$La_{0.7}Ca_{0.3}MnO_3/La_{0.3}Ca_{0.7}MnO_3$ superlattices

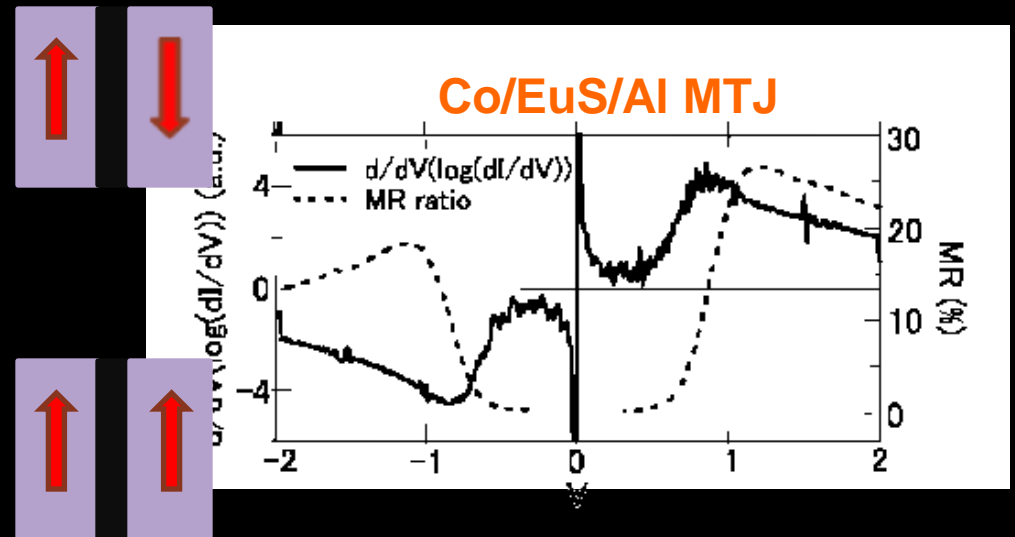
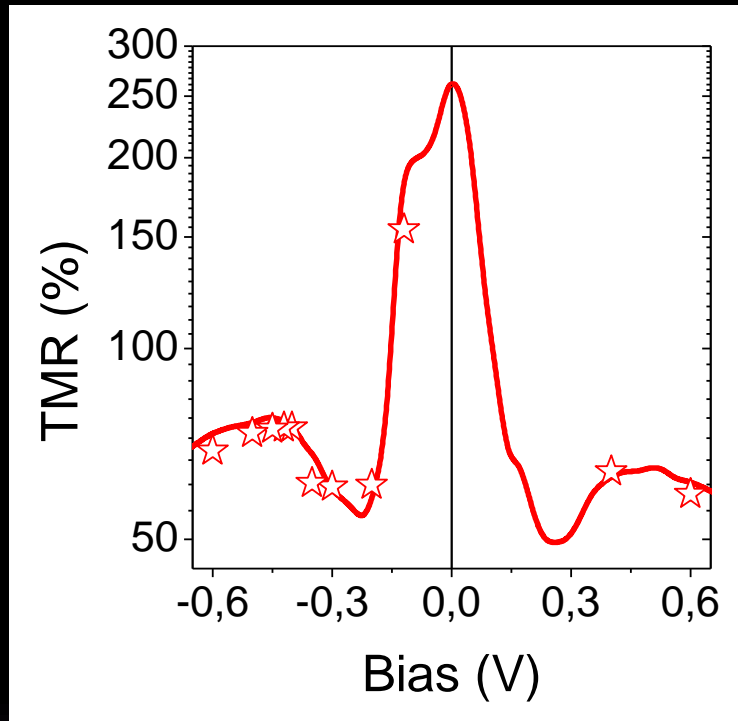
Polarized neutron reflectometry:



At low T (5 K) a finite ($1-2 \mu_B/\text{Mn}$) magnetization is present in the nominally AF barrier

$\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{La}_{0.3}\text{Ca}_{0.7}\text{MnO}_3/\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$

Bias dependence of tunneling MR in tunnel junctions

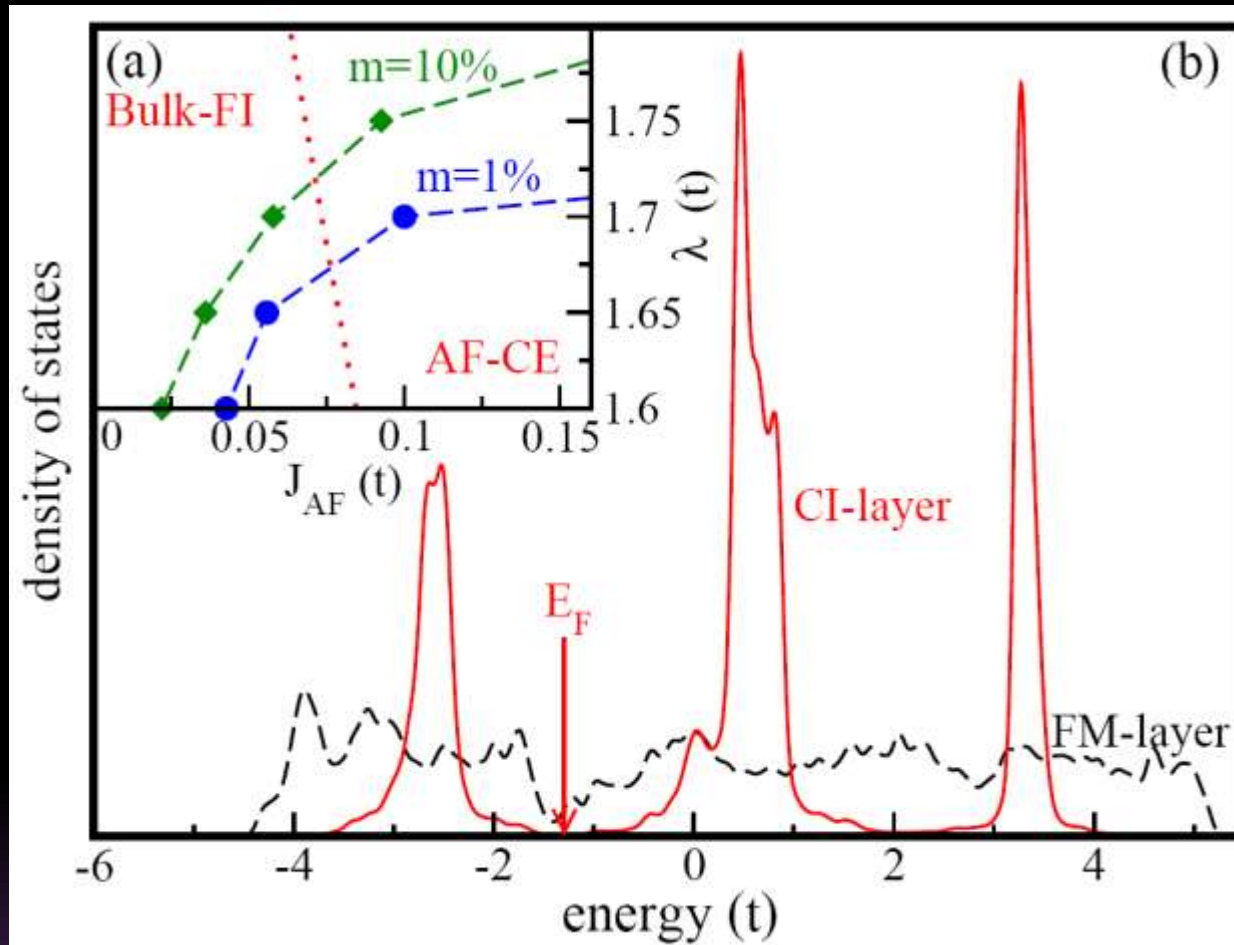


Nagahama et al,
PRL 99, 016602 (2007)

- ⊙ TMR first decreases with bias and then increases
- ⊙ Not the typical behavior in MTJs
- ➔ Reminiscent of spin-filter junctions

➔ **A ferromagnetic-like insulating state** is induced in the nominally antiferromagnetic barrier

Theory: $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$



- The interface is spin-canted (finite magnetic moment) and insulating.
- Magnetic moment depends on AF and Jahn-Teller (λ) couplings.

Conclusions

- ➔ Heterostructures of manganites constitute a great playground to study the interplay of different strongly correlated phases.
- ➔ A ferromagnetic and metallic interface is formed between two AF insulating manganites CaMnO_3 (band insulator) and $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ (strongly correlated insulator)

MJ Calderón, J. Salafranca, L. Brey, PRB 78, 024415

- ➔ FM metallic electrodes induce a FM insulating state in a nominally AF barrier. New approach to spin-filtering.

Z. Sefrioui, C. Visani, M.J. Calderón, K. March, C. Carrétéro, M. Walls, A. Rivera-Calzada, C. León, R. López Antón, T.R. Charlton, F.A. Cuéllar, E. Iborra, F. Ott, D. Imhoff, L. Brey, M. Bibes, J. Santamaría and A. Barthélémy, accepted in Advanced Materials (July 2010).