

(I)

# Surfaces and Interfaces: Correlated

Electron Sys Materials

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- How do the characteristic behaviors of correlated electron materials change at a new surface or interface (= material/vacuum int)
- Many questions: device engineering  $\rightarrow$  basic physics
- Ability to find answers - now within reach
- Still: more questions than answers  
more areas where the good question needs to be formulated.  
Here: present questions + a few basic concepts
- These lectures: mainly transition metal oxides

- ~~(I) Motivating Questions + Foundational Expts~~
- ~~(II) The polarization catastrophe~~
- ~~(III) The  $\text{LaTiO}_3 / \text{SrTiO}_3$  heterostructure~~
- ~~(IV) Colossal Magnetoresistance~~
- ~~(V) Prospects~~

- (I) The Questions
- (II) Some motivating experiments
- (III) Theory polarization catastrophe
- (IV) Theory
- (V) The  $\text{LaTiO}_3 / \text{SrTiO}_3$  heterostructure
- (VI) CMR heterostructures
- (VII) Prospects

The Questions

- Correlated electron materials: CTMO/
  - $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  - high  $T_c$
  - $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  - "half metal" (pol. cond. band)
    - charge, orbital, mag. order
    - "colossal" MR + other enhanced response
- $\text{V}_2\text{O}_3$  - metal insulator transition

General: "exotic" electronic phases  
enhanced response

~~Qn. how does this change near an interface~~  
~~Both "academic" and practical relevance~~

Physics: d-orbital. Starts  $5 \times$  degen.  
 $\Rightarrow$  can hold 10 el.

- <sup>+physics</sup> occupancy strongly affected by
  - ~~carrier density~~
  - Interaction effects:
    - $U_{dd} = E(N+1) + E(N-1) - 2E(N)$
    - Hund coupling (max spin state)
- Ligand field [split d-levels] @ lattice
- Hybridization (electron itinerancy)
- Carrier density  $\downarrow$

In many materials, different states close by in energy are finely balanced  
 $\Rightarrow$  even small changes  $\Rightarrow$  big differences

- What is different about surface/interface
  - Surface: lower coordination (1 direction electrons can't go)
  - Different interaction. [U dep. on environment] - Scattered
  - Different crystal symmetry (typically lower)

Rules of thumb:

- lower coordination: less KE  $\Rightarrow$  more ns
- vacuum: less screening  $\Rightarrow$  larger U
- lower sym: less fluct., easier to localize.

$\Rightarrow$  CVO prl.  
 $\Rightarrow$  Moore PRL

- Question not just academic

$$3(1-x) + 2(x) - 6 + [U_n] = 0 \Rightarrow \begin{cases} V_n = 3+x \\ n_d = 3+x \end{cases}$$

$\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ : Mn:  $\bar{n}$  cubic environment  
 $\equiv e_g \quad x^2-y^2 \quad 3z^2-r^2$

$\Rightarrow$  5 Mn d:  $\equiv t_{2g} \quad (d_{xy}, d_{xz}, d_{yz})$

Interactions such that  $4-x$  d  $e^-$  / Mn

3 in  $t_{2g}$ , max spin state  
 $(1-x)$  in  $e_g$ . Spin "slaked" to  $t_{2g}$  "core"  
 spin.

