Interfaces and Grain Boundaries of High Temperature Superconductors

from a theoreticians perspective

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(1) electrostatic interface tuning (SuFETs)

(2) nanomagnetism at interfaces of HTSCs

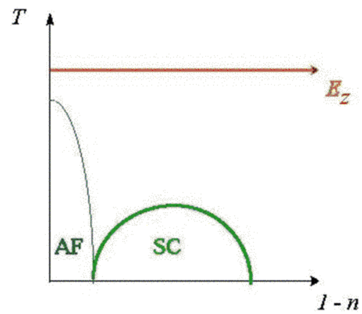
Why consider interfaces ?

- most devices are interface driven
- HTSC cables are not single crystals
  - grain boundaries may control the transport
- interfaces of correlated electronic systems may provide a new type of complexity; »reconstruction« of electronic states (?)

Electrostatic interface tuning (SUFETs)

theory:

Natalia Pavlenko
Verena Koerting
Qingshan Yuan
Peter Hirschfeld

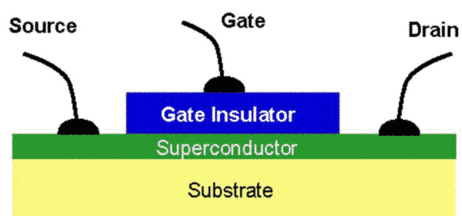


field doping

? instead of ?

chemical doping

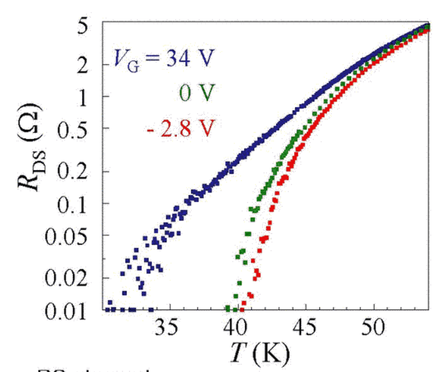
tune phase transitions electrostatically ?



experiment:

Jochen Mannhart
Gennadij Logvenov
Christof Schneider

Is electrostatic interface tuning feasible ?

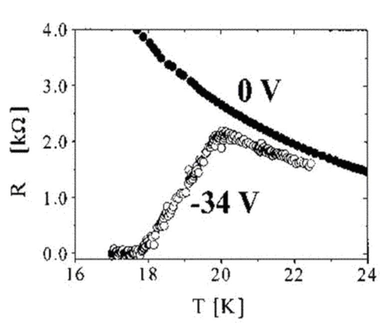


DS-channel:
8 nm polycrystalline $YBa_2Cu_3O_{7-d}$

gate barrier:
300 nm epitaxial $Ba_{0.15}Sr_{0.85}TiO_3$

- $YBa_2Cu_3O_{7-\delta}$, electric field across Kapton foils: fractional shifts in R_N of O(10^{-5}) (Fiory *et al.*, 1990)
- $YBa_2Cu_3O_{7-\delta}$, electric field across $SrTiO_3$ barriers with 4 x10^6 V/cm: major T_c shift (J. Mannhart, 1991, `96)
- T_c shifts of 10 K YBCO film on $SrTiO_3$ with 10 μC/cm² gate polarization (G. Logvenov, 2003)

insulator-superconductor transition observed in a $Nd_{1.2}Ba_{1.8}Cu_3O_7$ epitaxial film on $SrTiO_3$ substrate (A. Cassinese *et al.*, 2004)



Is electrostatic interface tuning feasible ?

- achieved areal carrier densities:
  0.01 — 0.05 carriers per unit cell

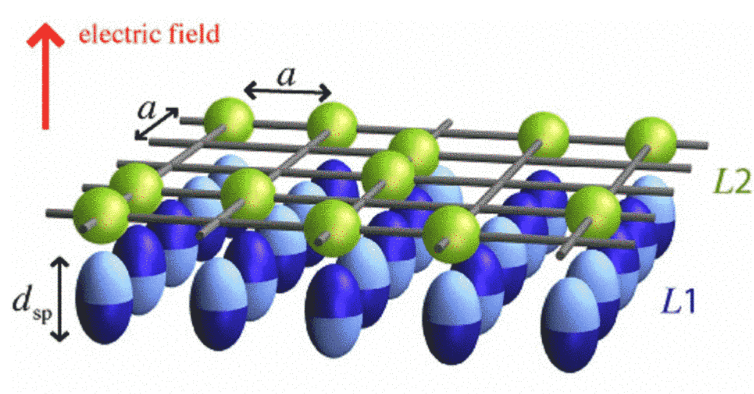
  → *limited by dielectric constant* **ε** *and breakdown field*
  for $SrTiO_3$ films: ε ~ 100 and breakdown ~ 10^8 V/m

- charge profile studied by Wehrli, Poilblanc & Rice (2001) and Pavlenko (unpublished)

  → *charge confined to surface layer when field doping the insulating state*
  ~ underdoped ~ 80 % , overdoping ~ 100 % in surface layer

electrostrostatic interface tuning is feasible
no fundamental objection to higher charge densities

Theoretical design of the interface

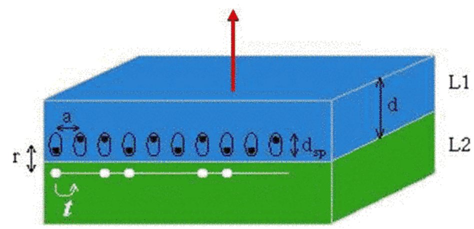


Theoretical design of the interface

electrostatic gate field

polarization of dielectric

accumulation of charge at interface



electric field energy: $\varepsilon_g = e d_{sp} E_z$

two-level systems: levels $p,\ s$

2D band: bandwidth $8t$

single particle processes:

$$H_t = -t \sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}{}^\dagger c_{j,\sigma}$$

$$H_{2l} = \frac{1}{2}\Delta_{sp} \sum_i (p_i{}^\dagger p_i - s_i{}^\dagger s_i)$$

$$H_{ext} = \varepsilon_g \sum_i (p_i{}^\dagger s_i + s_i{}^\dagger p_i)$$

interaction between charge excitations in L1 and L2:

$$H_{int} = V_{sp} \sum_{i,\sigma} c_{i,\sigma}{}^\dagger c_{i,\sigma}\ (p_i{}^\dagger s_i + s_i{}^\dagger p_i)$$

interaction between charge carriers in L2:

$$H_{e-e} = U \sum_i c_{i,\uparrow}{}^\dagger c_{i,\uparrow}\ c_{i,\downarrow}{}^\dagger c_{i,\downarrow}$$

$H_t + H_{2l} + H_{ext} + H_{int} + H_{e-e}$

interaction between metallic charge carriers and (polarized) two-level systems

$$H_{int} = V_{sp} \sum_{i,\sigma} c_{i,\sigma}{}^\dagger c_{i,\sigma}\ (p_i{}^\dagger s_i + s_i{}^\dagger p_i) \qquad V_{sp} \sim \frac{e^2 d_{sp}}{r^2}$$

$$= V_x \sum c^\dagger c\ \ (S^+ + S^-) \ + \ V_z \sum c^\dagger c\ \ S^z$$

with

$$V_x = \frac{V_{sp}}{2} \frac{\Delta_{sp}}{\sqrt{\varepsilon_g{}^2 + (\frac{1}{2}\Delta_{sp})^2}} \qquad V_z = 2V_{sp} \frac{\varepsilon_g}{\sqrt{\varepsilon_g{}^2 + (\frac{1}{2}\Delta_{sp})^2}}$$

V_x (virtual) transitions driven by field of nearest charge carrier
⟹ induce pairing

V_z interaction of field induced dipoles with the 2D charge carriers
⟹ repulsive term in pairing channel

Steps towards an approximate solution

1. bosonization (Holstein-Primakoff)

$$S_j^+ \to b_j \quad , \quad S_j^- \to b_j^\dagger \quad , \quad S_j^z \to \frac{1}{2} - b_j^\dagger b_j$$

not exact but correct for negligible inversion:

$$\langle b_j^\dagger b_j \rangle \ll 1$$

2. generalized Lang-Firsov transformation

$$\tilde{H} = U_{LF}{}^\dagger H U_{LF}$$

purpose of unitary transformation:

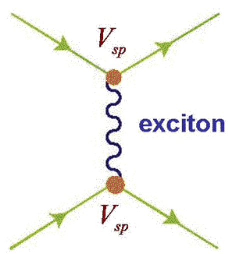
$$V_x c^\dagger c (b + b^\dagger) \to V_{eff} c^\dagger c^\dagger c c$$

Induced pairing (at U=0)

second order perturbation theory for zero field:

$$V_{eff} \big|_{\text{zero field}} = 2 \frac{V_{sp}^2}{\Delta_{sp}}$$

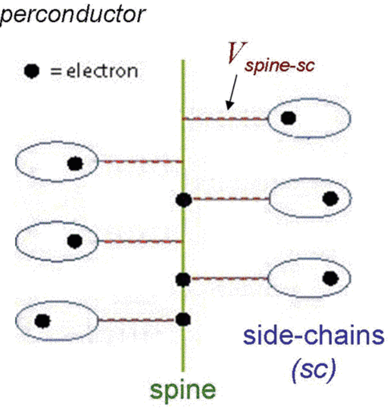
positive: attractive interaction



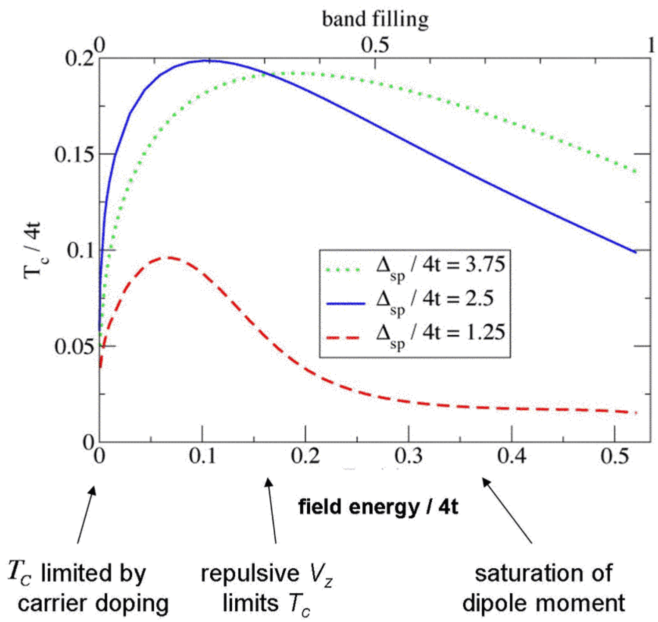
Possibility of Synthesizing an Organic Superconductor
(W. A. Little, 1964)

spine: metallic
half-filled band ε_k
(polyene chain)

side-chains: charge oscillation
with low-lying excited state Δ_{sc}



Field dependence of T_C (at U=0)



maximum in T_c for intermediate fields

$$\frac{\Delta_{sp}^{\text{opt}}}{4t} \approx 2.5$$

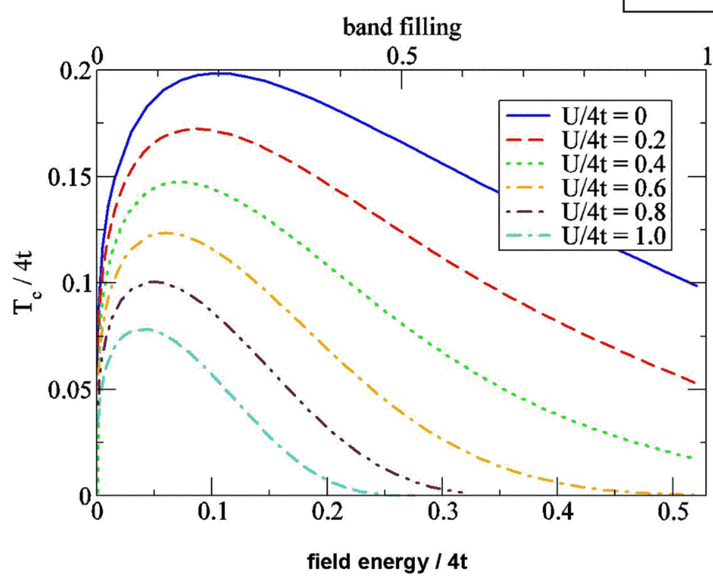
not strongly dependent on other parameters like V_{sp} and ε

e.g. CT excitations in $SrTiO_3$

(V. Koerting, Q. Yuan, P. Hirschfeld, T.K., and J. Mannhart, PRB **71**, 104510 (2005))

Including a repulsive interaction in the metallic layer

$$H_{e-e} = U \sum_i c_{i,\uparrow}^{\dagger} c_{i,\uparrow} \, c_{i,\downarrow}^{\dagger} c_{i,\downarrow}$$



(V. Koerting, Q. Yuan, P. Hirschfeld, T.K., and J. Mannhart, PRB **71**, 104510 (2005))

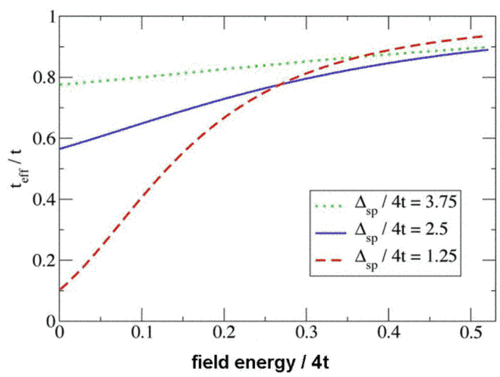
Strong coupling: mapping onto a *t-J* model

renormalization of nearest neighbor spin exchange
through charge transfer excitons $(U \approx 8t,\ t'/t \approx -0.3,\ V_{sp}/\Delta_{sp} \approx 1)$:

$\Delta U / U \approx -0.2 \quad \rightarrow \quad J_{\text{eff}} / J \approx 1.07$ insignificant

$t_{\text{eff}} / t \approx 0.7 \quad \rightarrow \quad J_{\text{eff}} / J \approx 0.5$ major correction

band renormalization at T_C



coupling to excitons:

delocalization with increasing field

Inclusion of phonon modes

(N. Pavlenko, T.K., cond-mat/0505714)

closer to realistic modelling, a further step in complexity:

$$H = H_{t,t'} + H_{2l} + H_{ext} + H_{int} + H_{e-e} + H_{\text{pol}}$$

coupling to polar phonons at the interface

disorder still not implemented !

$SrTiO_3$: soft TO_1-mode at $\omega_{TO} \approx$ 50–80 cm^{-1}

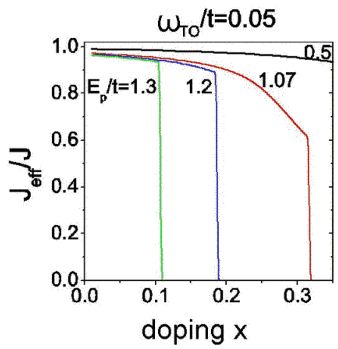
$$H_{\text{pol}} = \hbar\omega_{TO} \sum_i b_i^\dagger b_i - \gamma \sum_{i\sigma} (1 - n_{i\sigma})(b_i^\dagger + b_i)$$

where

$\gamma = \sqrt{\hbar\omega_{TO} E_p}$ is the hole-phonon coupling $\gamma \approx 0.01 - 0.1$ eV

E_p is the polaron binding energy $E_p / \hbar\omega_{TO} \approx 0.1 - 5$

Strong coupling: superconductor-insulator transition



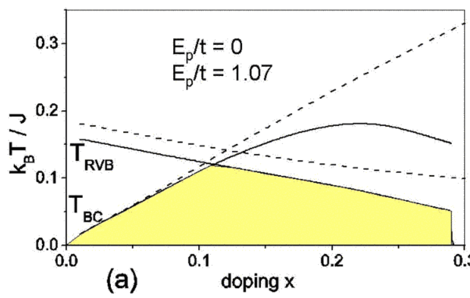
coupling to phonons :

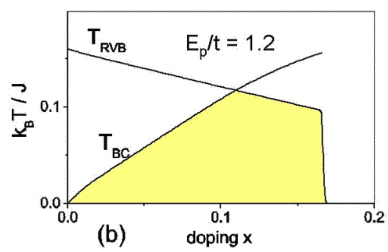
localization with increasing doping

similar evaluation for the CMR-manganites
compare: Röder, Zang, and Bishop (PRL 1996)

double exchange ↔ excitonic narrowing
JT phonon ↔ soft phonon mode

- slave-boson evaluation (with d-wave pairing):





Strong coupling: superconductor-insulator transition

coupling to phonons :

localization with increasing doping

coupling to excitons:

delocalization with increasing field

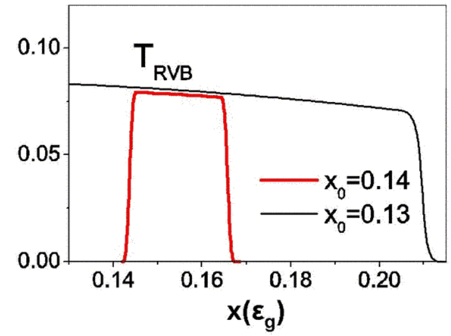
→ transition not only depends on the overall dopping
but also on the details of chemical versus field doping

Strong coupling: reentrant behavior

- the phase diagram now depends on

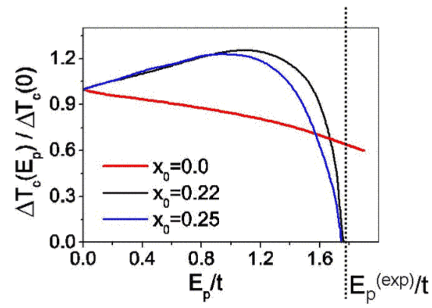
  doping at zero field x_0
  and
  the field doping $x(\varepsilon_g)$

  field-induced reentrant behavior:



- observed (field-induced) T_c shift in HTSC cuprate films depends on doping:

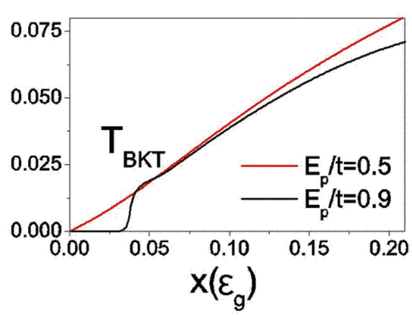
  in underdoped films sizable shift
  whereas
  in overdoped films (nearly) no shift



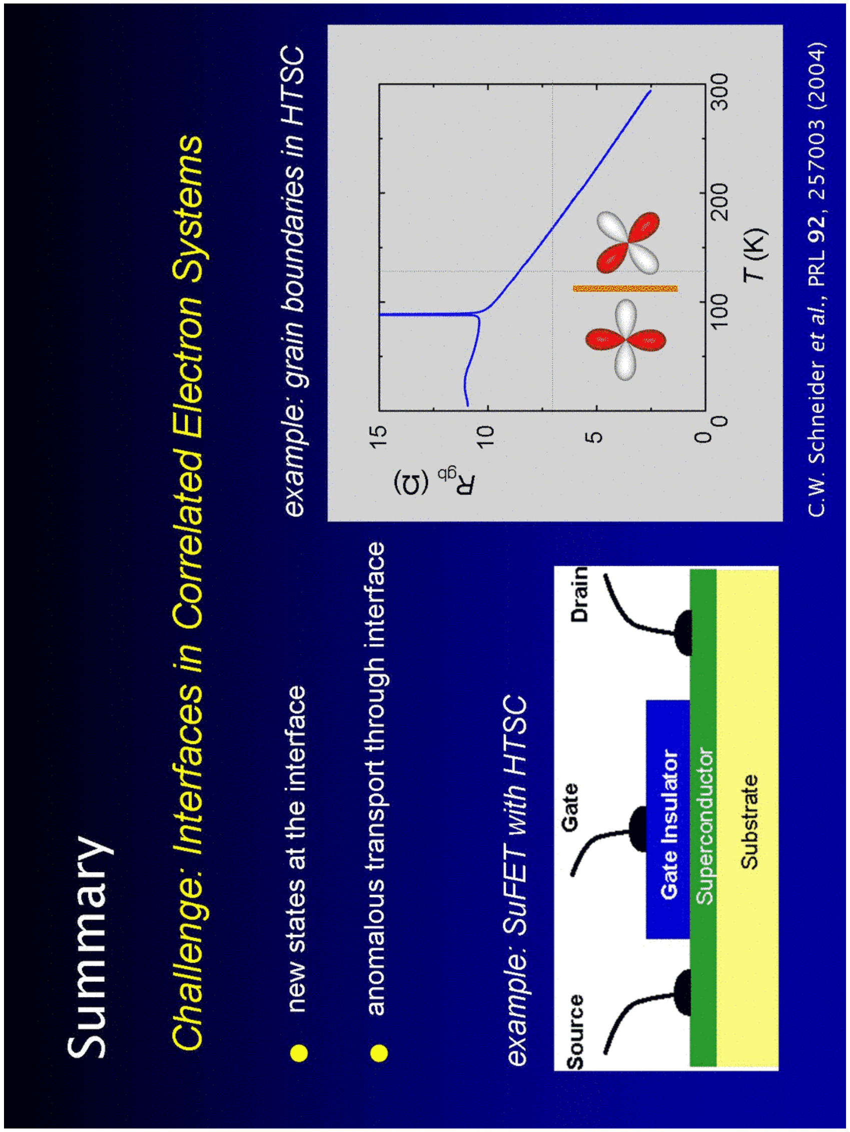
BKT transition

2D systems: Berezinskii-Kosterlitz-Thouless transition (BKT)

- T_{BKT} always smaller than T_{BKT}
- T_{BKT} increases nonlinearly with doping, due to interface coupling (cf. with experiments by Walkenhorst *et al.*, PRL,1992)



[evaluation similar to Kim & Carbotte, 2002]


Summary
Challenge: Interfaces in Correlated Electron Systems
new states at the interface
anomalous transport through interface
example: grain boundaries in HTSC
R_{gb} (Ω)
T (K)
C.W. Schneider et al., PRL 92, 257003 (2004)
example: SuFET with HTSC
Source
Gate
Drain
Gate Insulator
Superconductor
Substrate