Electric breakdown near first-order Mott transitions

Michele Fabrizio (SISSA)

SISSA
International School for Advanced Studies

European Research Council
FIRSTORM

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Outline

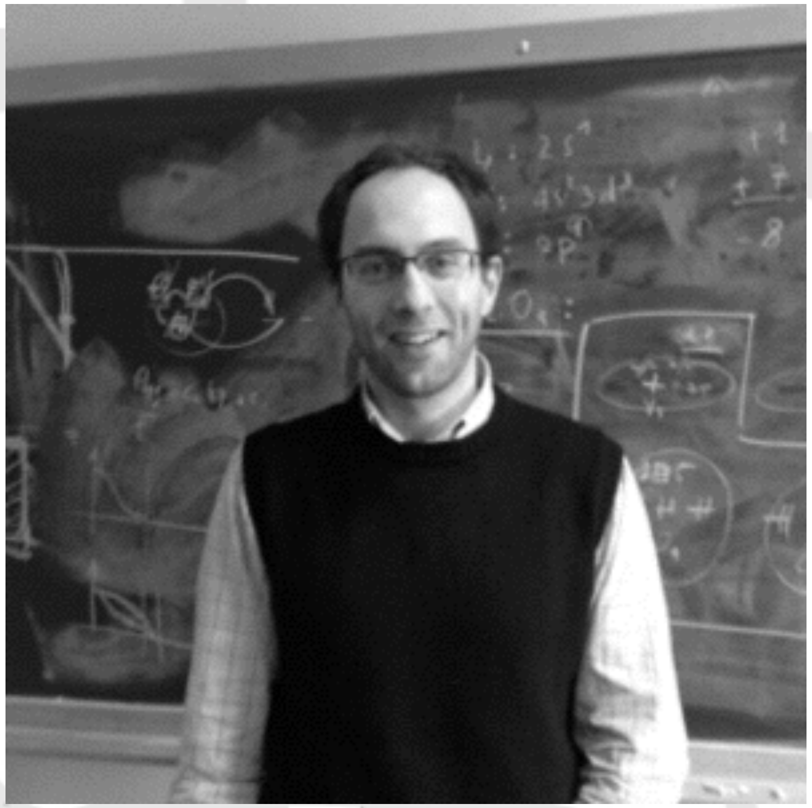
* Motivation: recent experiments on narrow-gap Mott insulators highlight the role played by the ubiquitous first-order nature of Mott transitions

* The importance of being first order: unconventional non-equilibrium behaviour

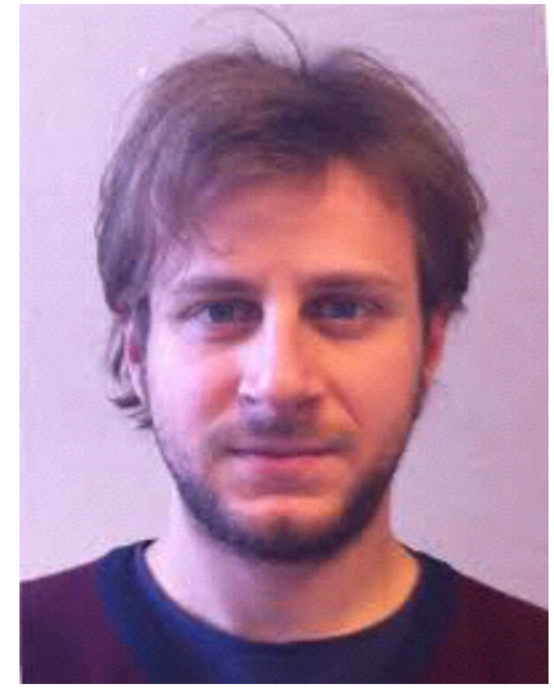
* A case study: non-Zener electric breakdown in a simple model of a d-d Mott insulator

* Conclusions

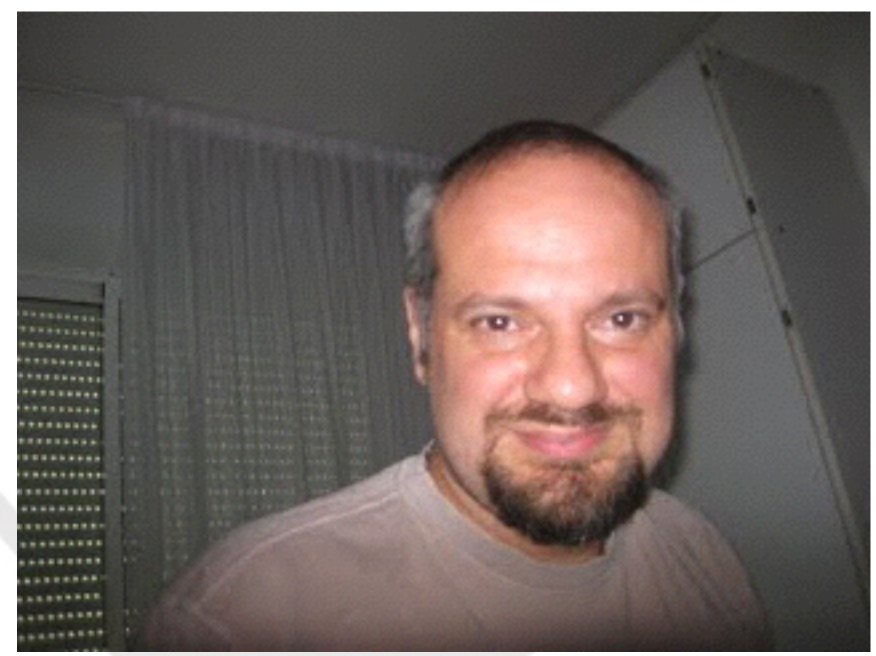
in collaboration with:



Adriano Amaricci (SISSA)



Giacomo Mazza (École Polytechnique)



Massimo Capone (SISSA)

arXiv:1602.03138
(to appear in PRL)

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at equilibrium ...

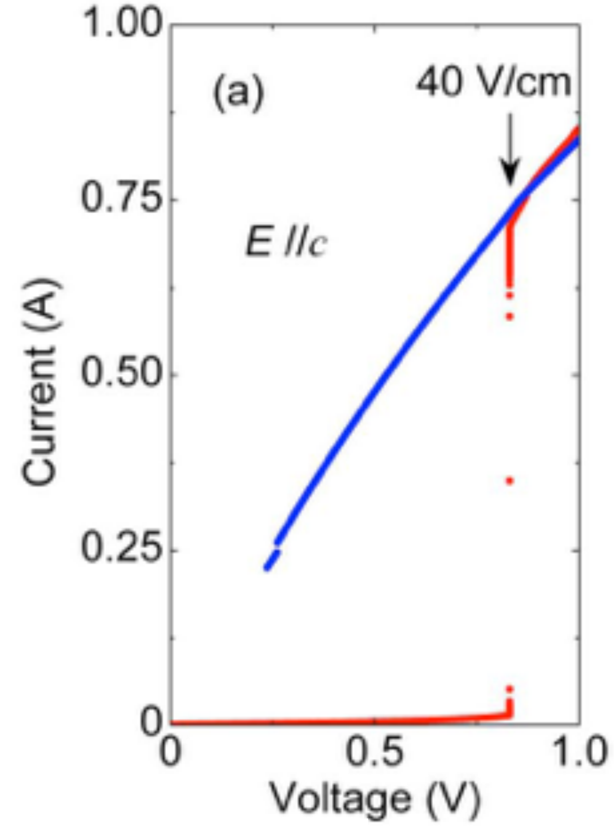
- Conventional band insulators: **boring**!!!
- Mott insulators: **exciting**!!!! Many interesting phenomena arise: high T_c superconductivity upon doping, CMR, etc...

Have Mott insulators still surprises in store also away from equilibrium that band insulators do not have?

SCIENTIFIC REPORTS | 3 : 2536 | DOI: 10.1038/srep02536

Electric-field-induced metal maintained by current of the Mott insulator Ca_2RuO_4

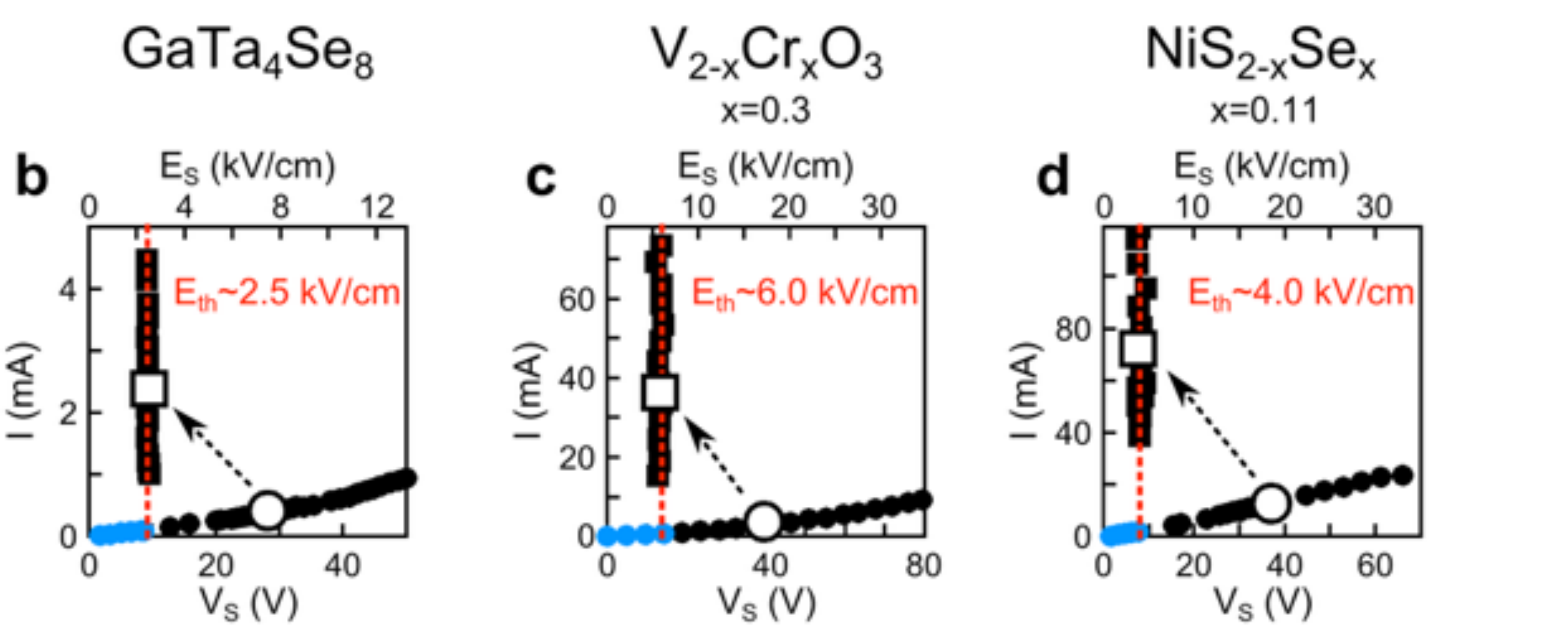
Fumihiko Nakamura[1], Mariko Sakaki[1], Yuya Yamanaka[1], Sho Tamaru[1], Takashi Suzuki[1] & Yoshiteru Maeno[2]



ADVANCED MATERIALS
www.advmat.de
[25, 3222 (2013)]
MaterialsViews
www.MaterialsViews.com

Universal Electric-Field-Driven Resistive Transition in Narrow-Gap Mott Insulators

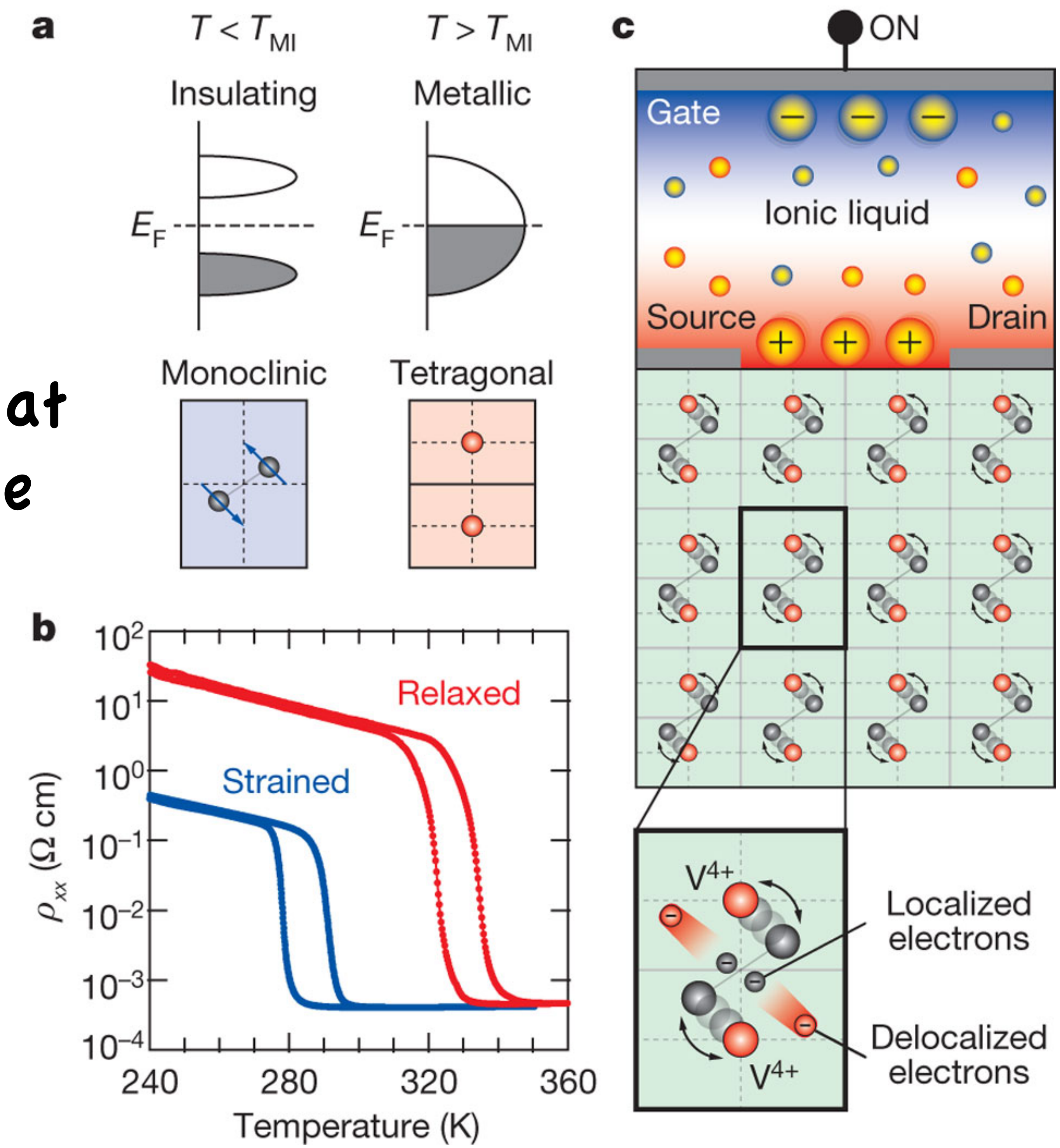
Pablo Stoliar, Laurent Cario, Etiene Janod, Benoit Corraze, Catherine Guillot-Deudon, Sabrina Salmon-Bourmand, Vincent Guiot, Julien Tranchant, and Marcelo Rozenberg**



the threshold electric field is orders of magnitude smaller than its estimate based on the Landau-Zener breakdown mechanism, which is around MeV/cm

The first-order metal–insulator transition in VO_2.

double-layer transistor formed at a solid-electrolyte interface



M Nakano *et al.* *Nature* **487**, 459-462 (2012) doi:10.1038/nature11296

LETTER

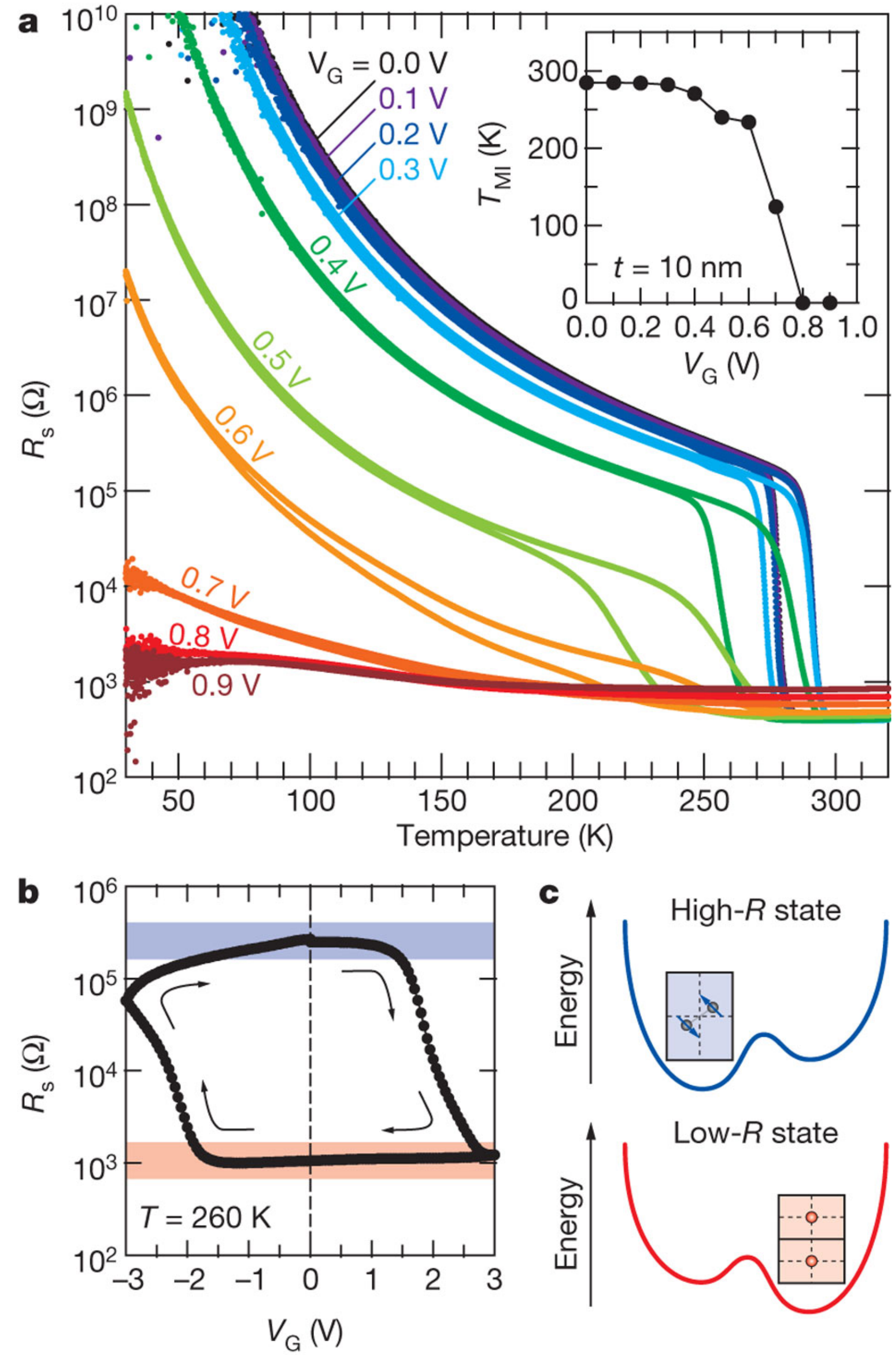
doi:10.1038/nature11296

Collective bulk carrier delocalization driven by electrostatic surface charge accumulation

M. Nakano[1], K. Shibuya[1]†, D. Okuyama[1], T. Hatano[1], S. Ono[1,2], M. Kawasaki[1,3], Y. Iwasa[1,3] & Y. Tokura[1,3]

M Nakano *et al.* *Nature* **487**, 459-462 (2012) doi:10.1038/nature11296

several layers turn metallic at the same time: wetting phenomenon?



APPLIED PHYSICS LETTERS 104, 023507 (2014)

Gate-tunable gigantic lattice deformation in VO_2

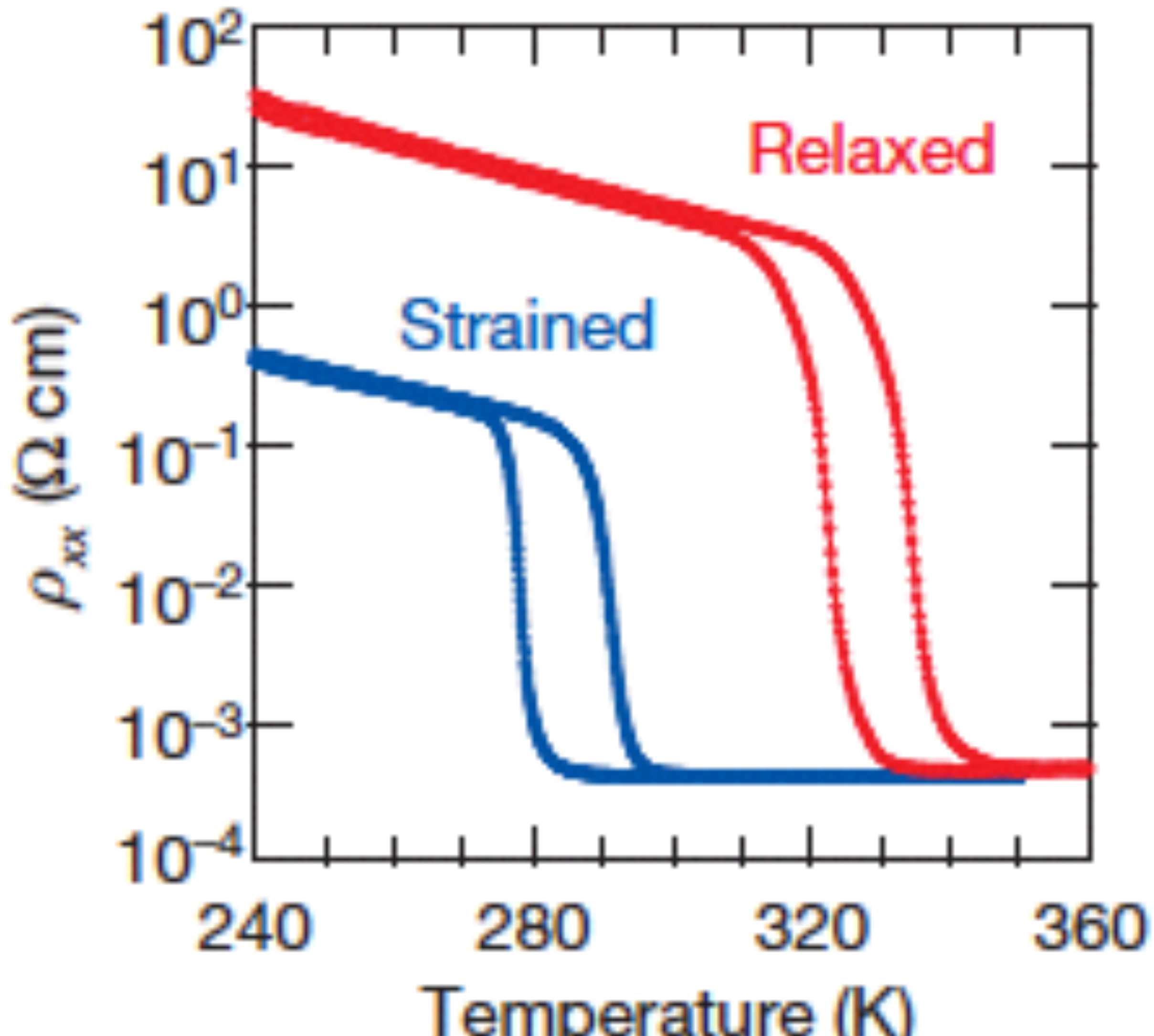
D. Okuyama,[1,a),b)] M. Nakano,[1,2,a),b)] S. Takeshita,[3] H. Ohsumi,[3] S. Tardif,[3] K. Shibuya,[4,c)] T. Hatano,[1] H. Yumoto,[5] T. Koyama,[5] H. Ohashi,[5] M. Takata,[3,5] M. Kawasaki,[1,6] T. Arima,[1,3,7] Y. Tokura,[1,6] and Y. Iwasa[1,6,b)]

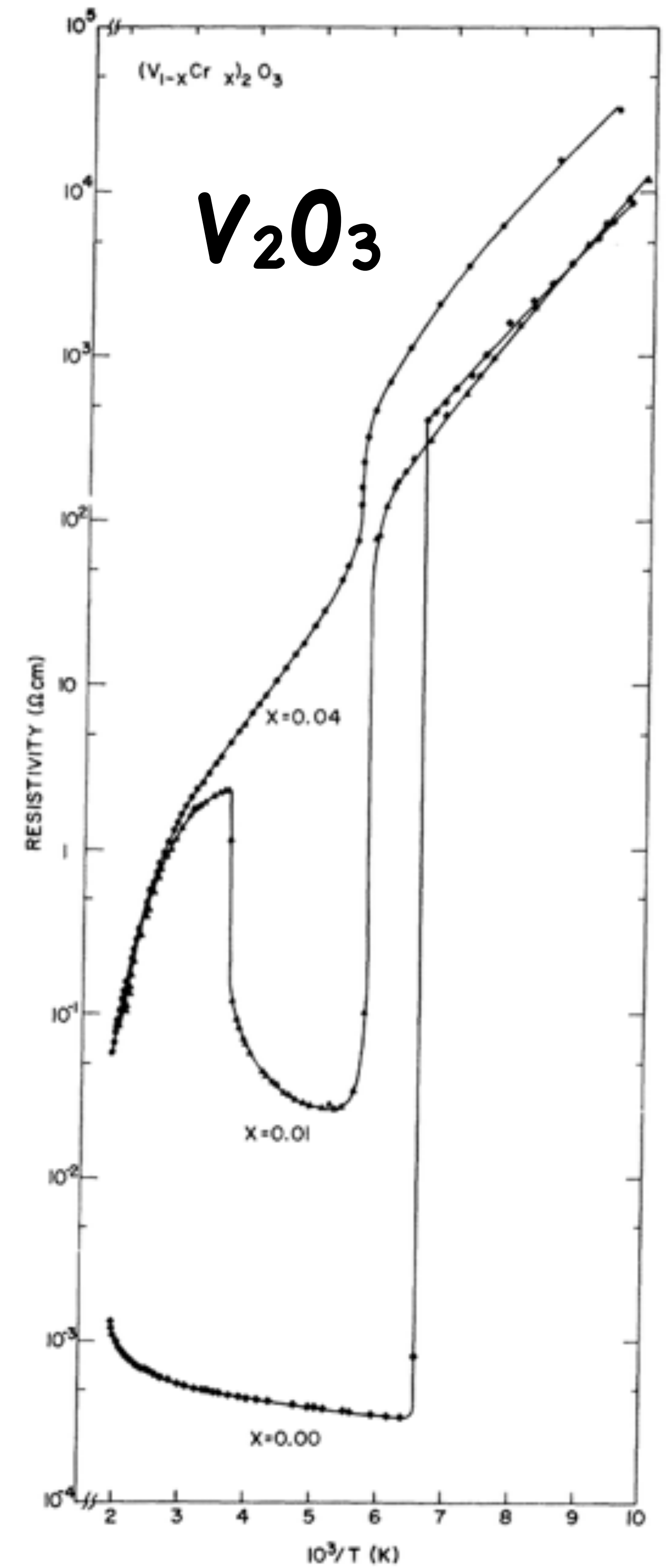
⋮

gate voltages (V_G). Moreover, it turned out that an electrically induced conducting channel is extended to an entire region of the 70-nm thick film along *c*-axis direction beyond the fundamental electrostatic screening length, which is in marked contrast to conventional FETs that have a two-dimensional conducting channel. We have attributed these phenomena to

✓ indeed, all known Mott transitions are strongly first order!

VO_2

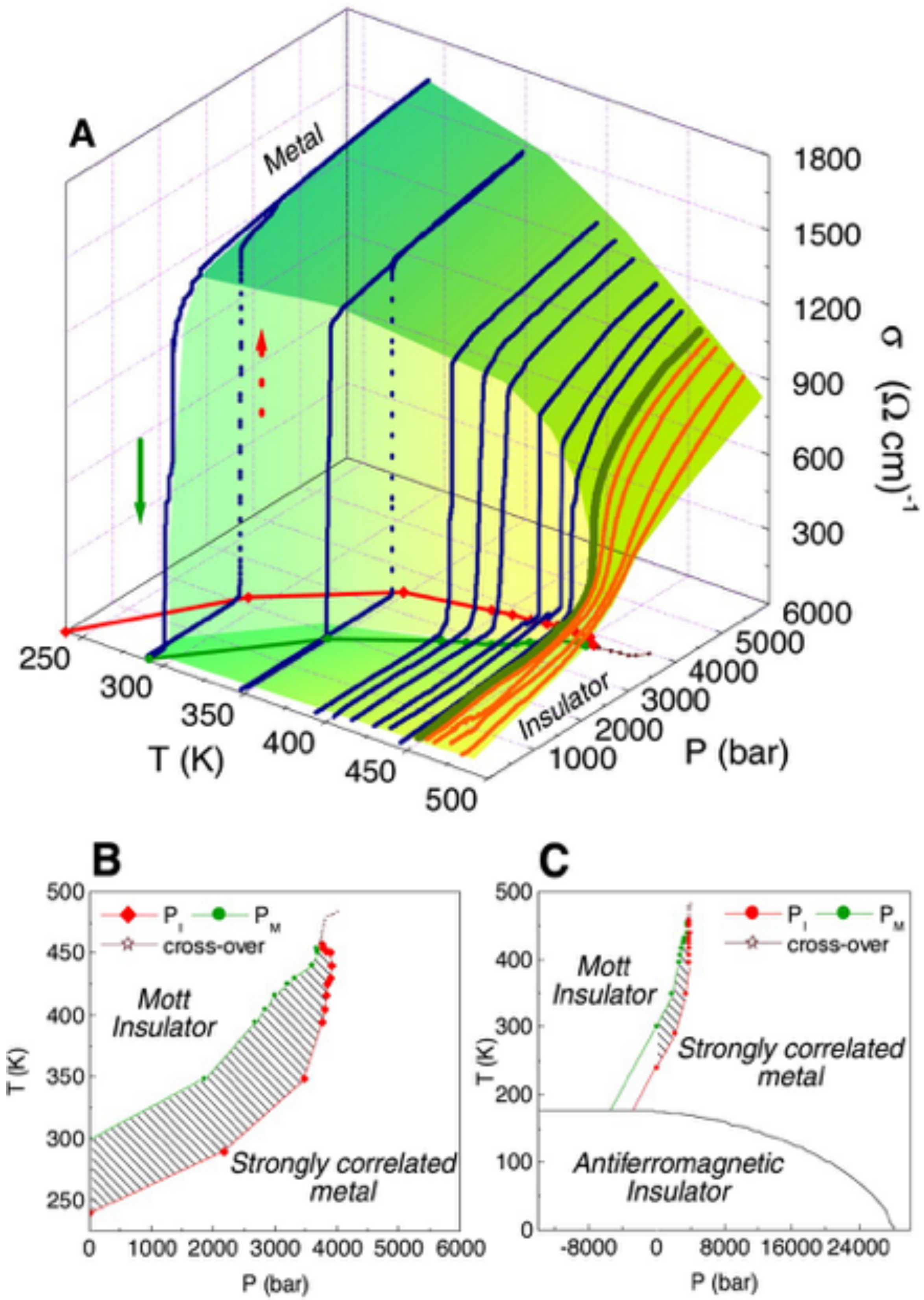




Universality and Critical Behavior at the Mott Transition

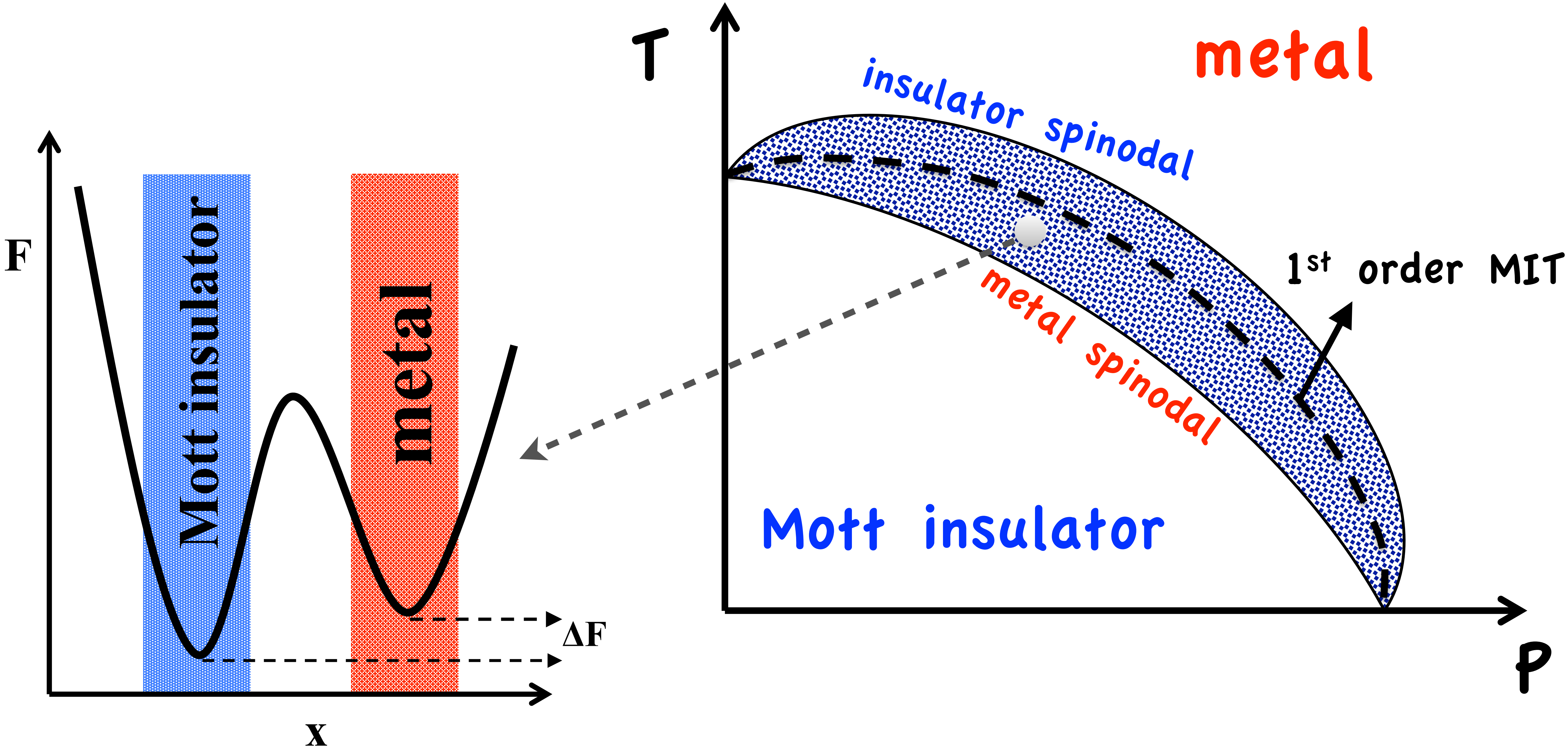
www.sciencemag.org SCIENCE VOL 302 3 OCTOBER 2003

P. Limelette,[1*] A. Georges,[1,2] D. Jérome,[1] P. Wzietek,[1]
P. Metcalf,[3] J. M. Honig[3]

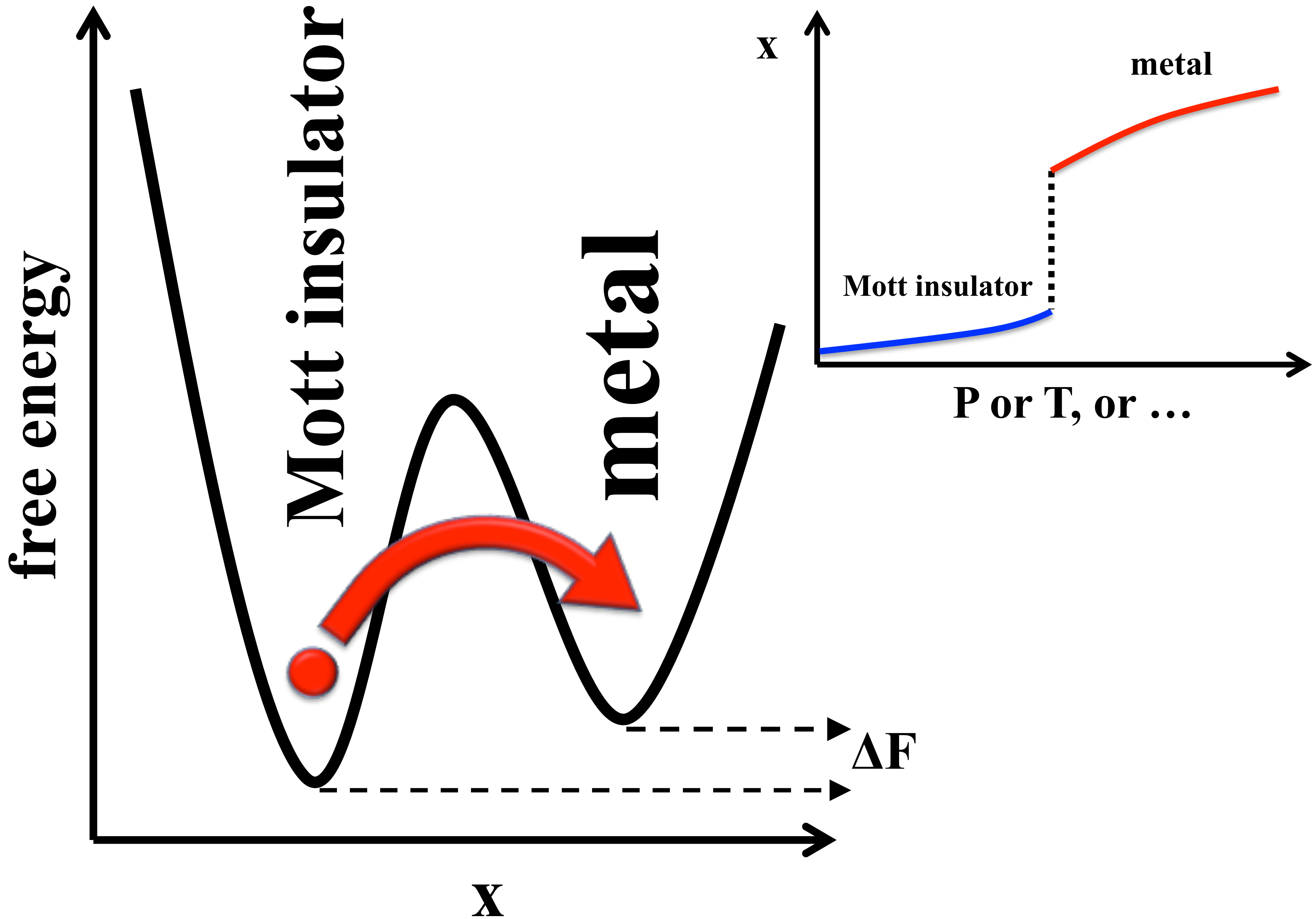


with quite sizeable coexistence domains

Is the ubiquitous first-order character just a secondary phenomenon, not worth paying any attention to, or rather a relevant aspect to be studied and exploited?

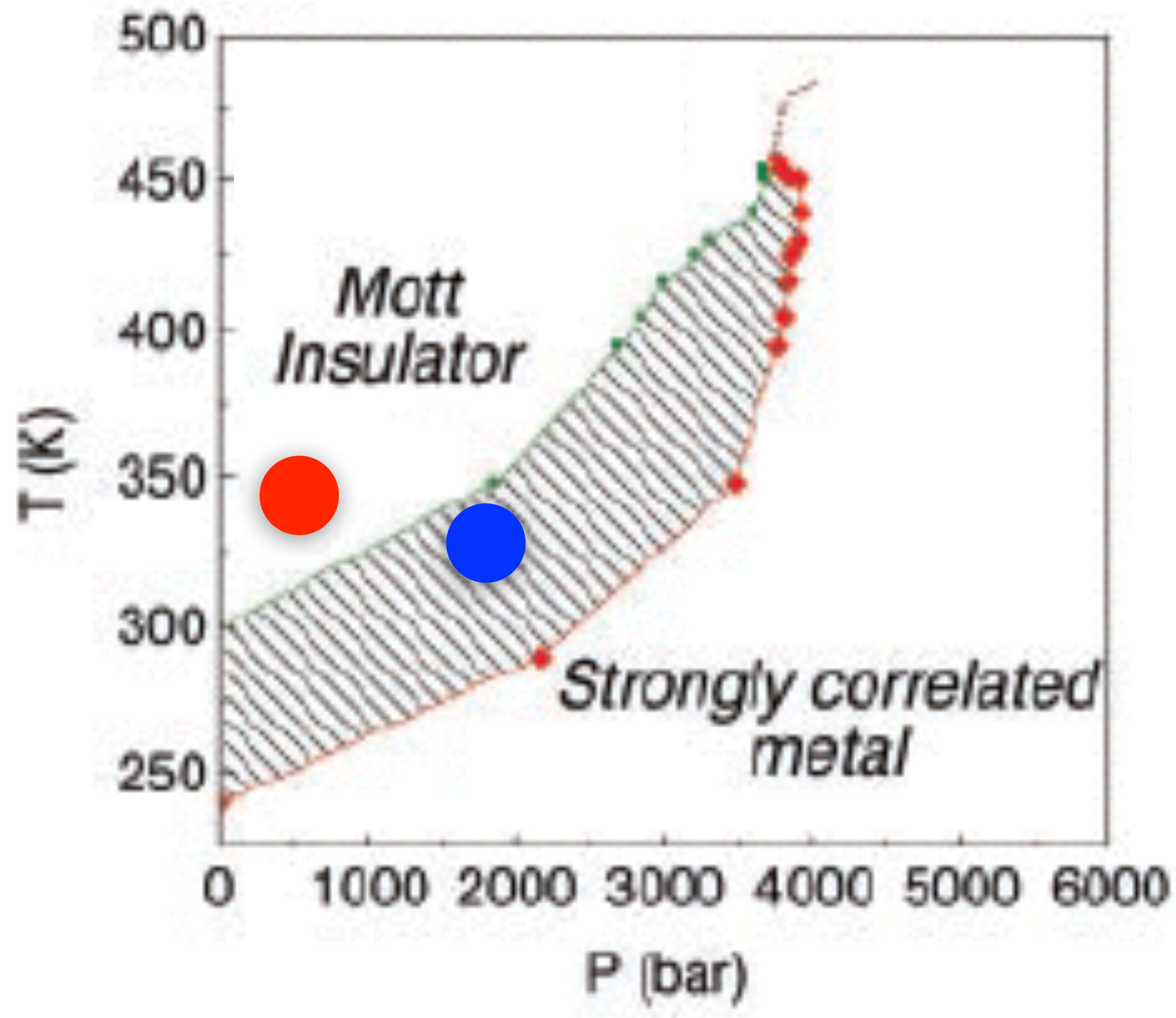


Near a first order Mott transition one encounters the unprecedented situation of a stable insulator that coexists with a metastable metal not at extreme pressure/temperature/etc... conditions!

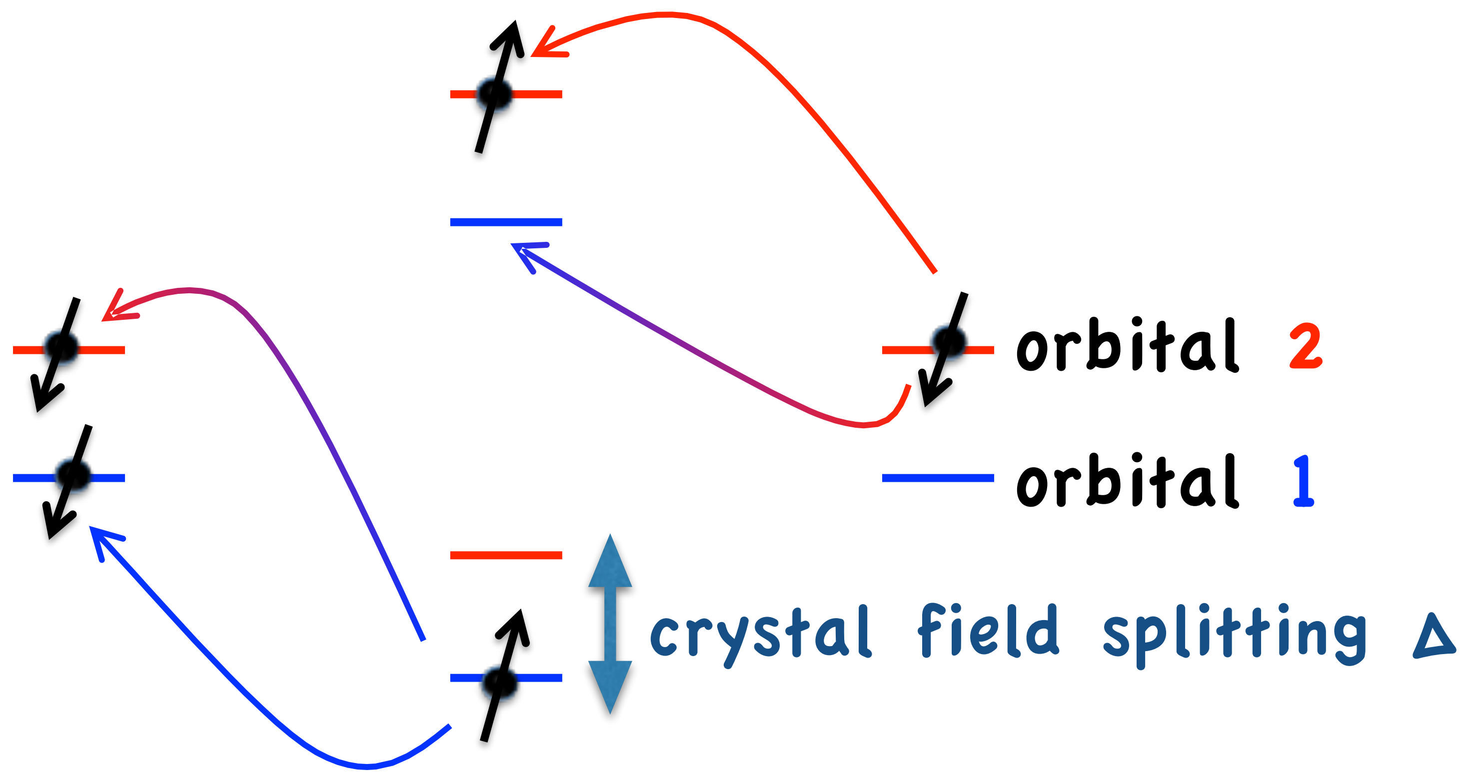


An external field **E** that couples to the state variable x, $\delta H = - E\, x$, might trigger a transition into the metastable metal phase

Question: does the electric breakdown of a Mott insulator depend whether the system is inside or outside insulator-metal coexistence?



the simplest modelling of a d-d Mott insulator: a Hubbard model of two crystal-field split bands at half-filling

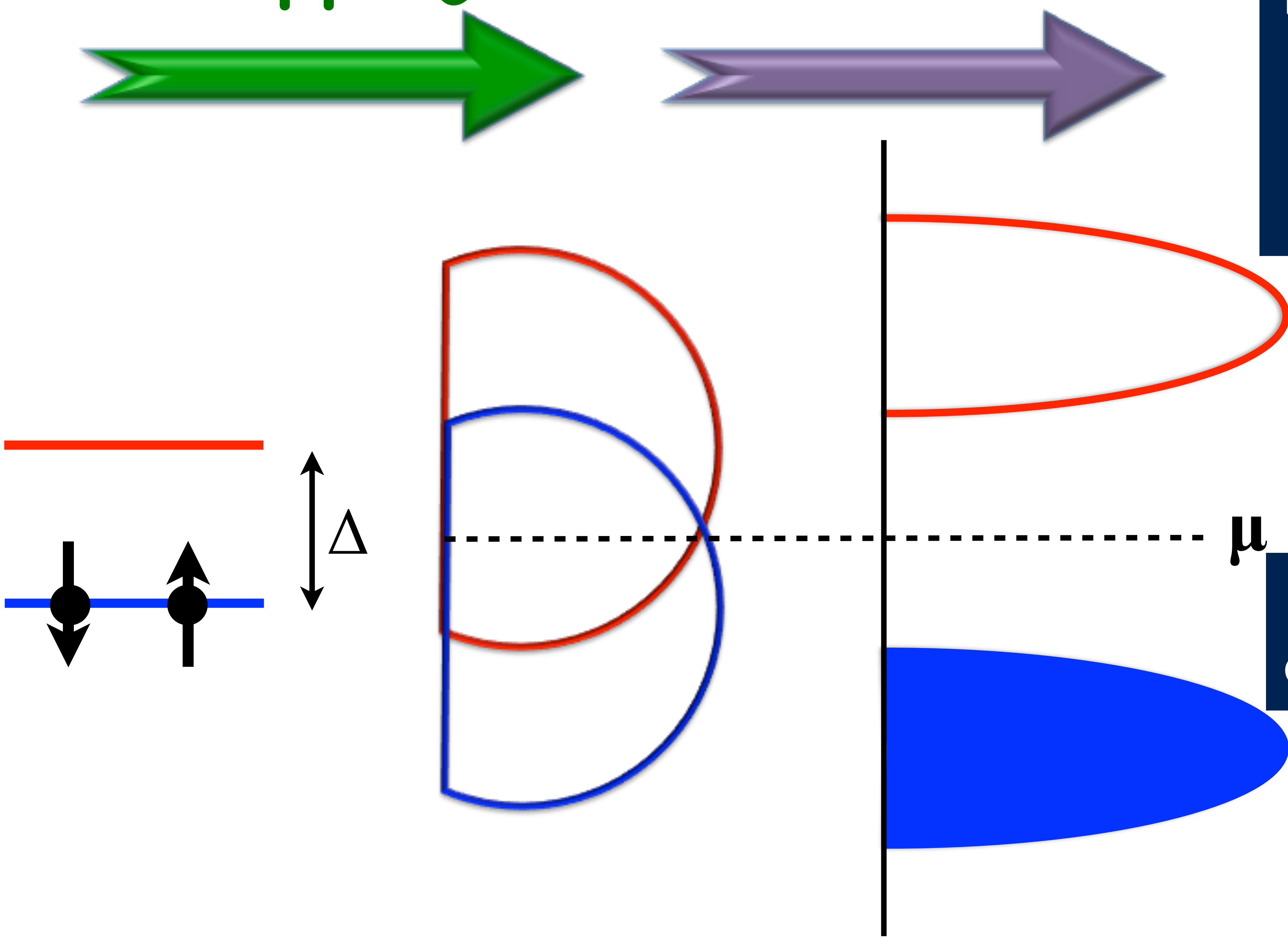


+ **Hubbard U**

favouring 2 electrons per site

$$\mathcal{H} = \sum_{\mathbf{R}\mathbf{R}',\sigma}\,\sum_{a,b=1}^{2} c^\dagger_{\mathbf{R}\,a\sigma}\, t^{ab}_{\mathbf{R}\mathbf{R}'}\, c_{\mathbf{R}'\,b\sigma} - \frac{\Delta}{2}\sum_{\mathbf{R}}\left(n_{\mathbf{R}\,1} - n_{\mathbf{R}\,2}\right) + \frac{U}{2}\sum_{\mathbf{R}}\left(n_{\mathbf{R}} - 2\right)^2$$

What do we expect?

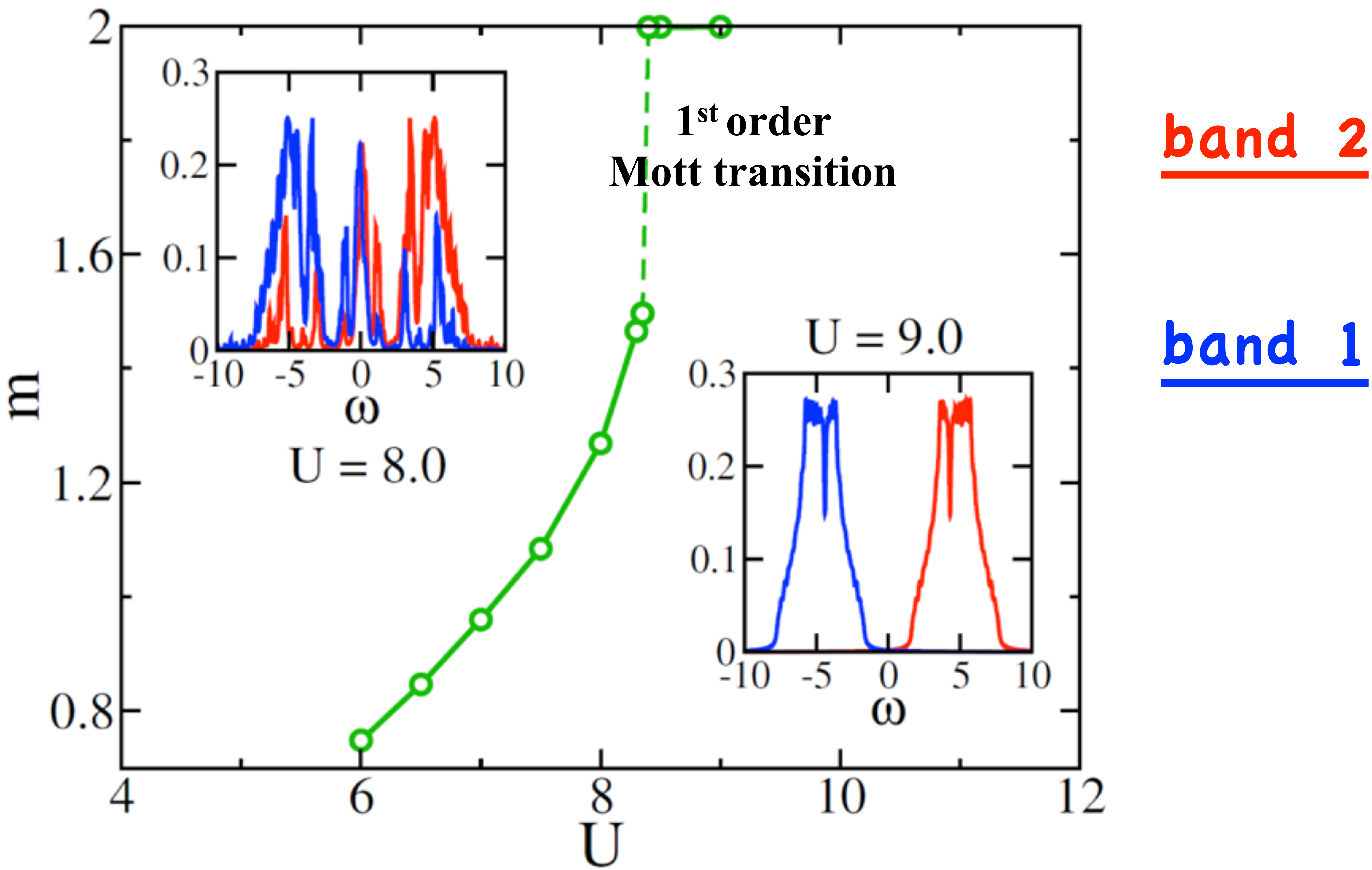


the interaction has two effects: it shrinks the bands and makes occupied and unoccupied states repel each other

the crystal field effectively increases

$$\Delta \to \Delta_* > \Delta$$

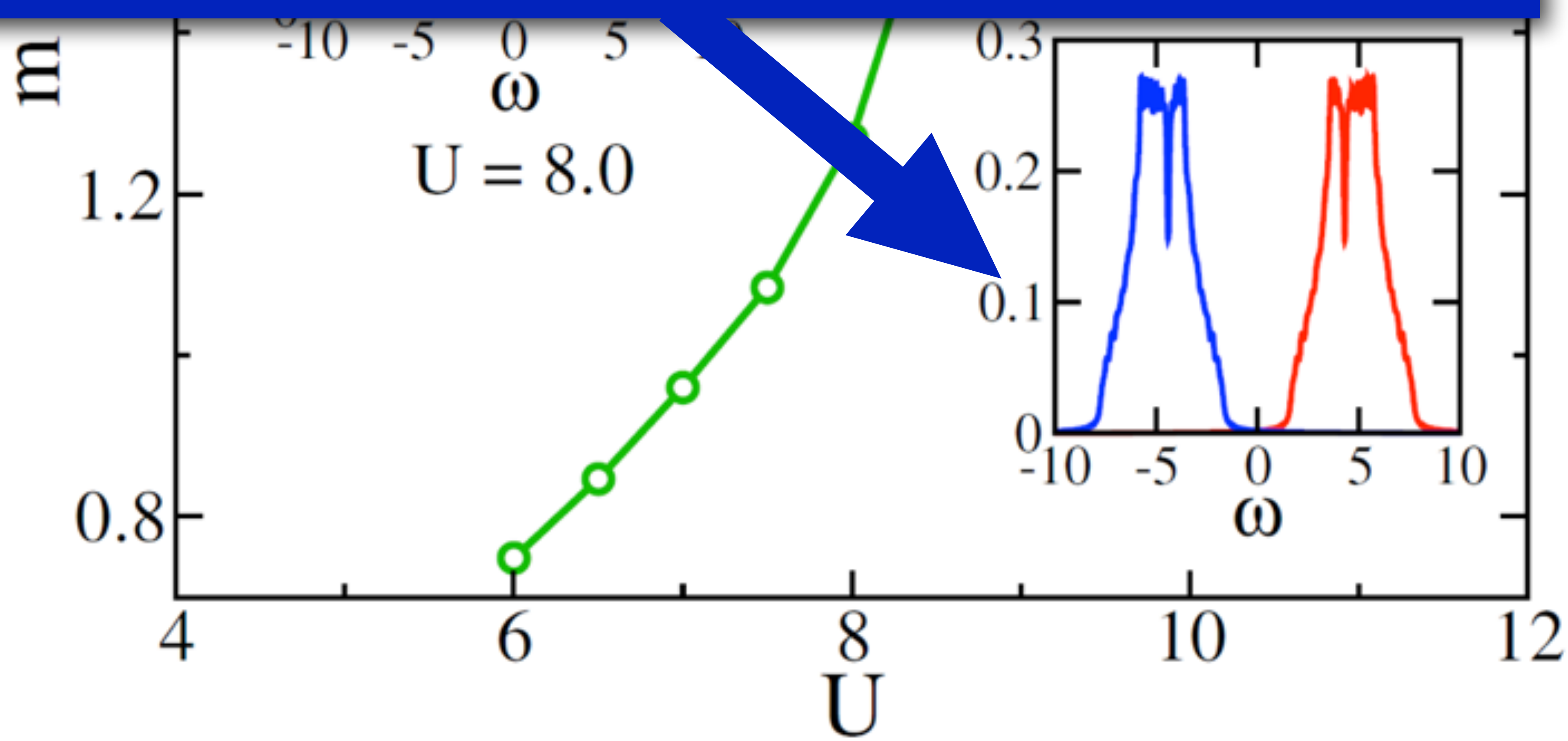
DMFT phase diagram



m = (occupation band 1) - (occupation band 2)

DMFT phase diagram

A Mott insulator disguised as a conventional band insulator!
(not so different from Goodenough's view of insulating VO_2)

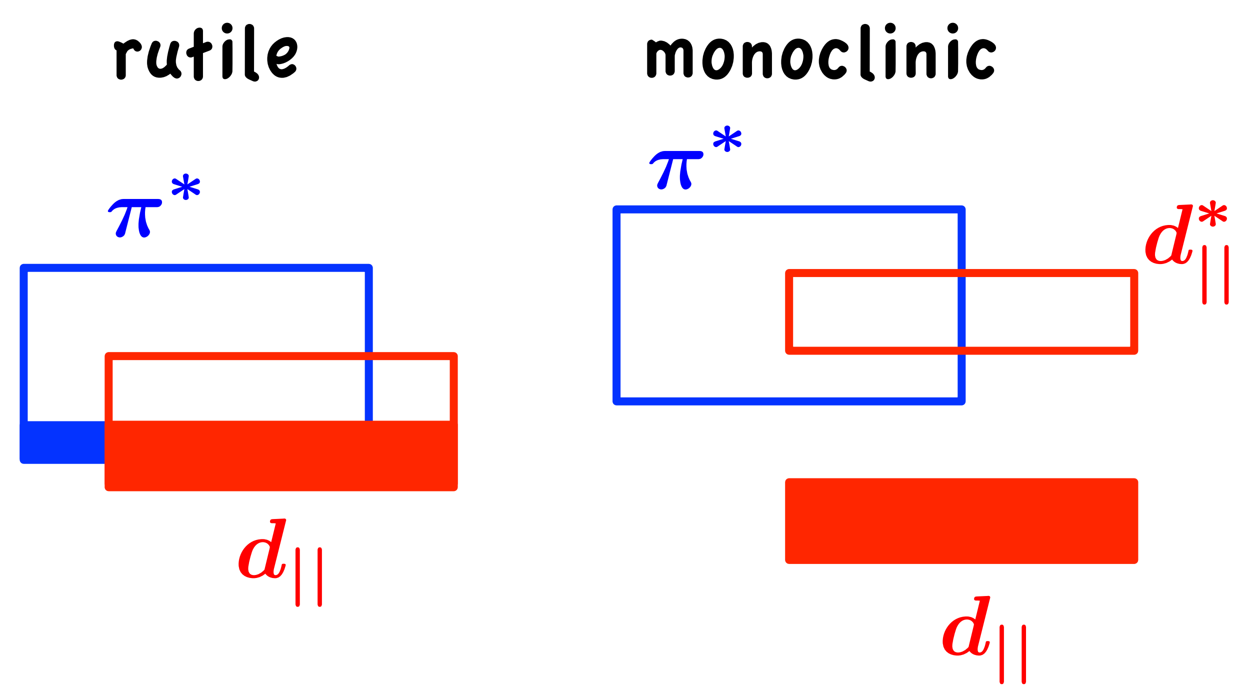


band 2

band 1

m = (occupation band 1) - (occupation band 2)

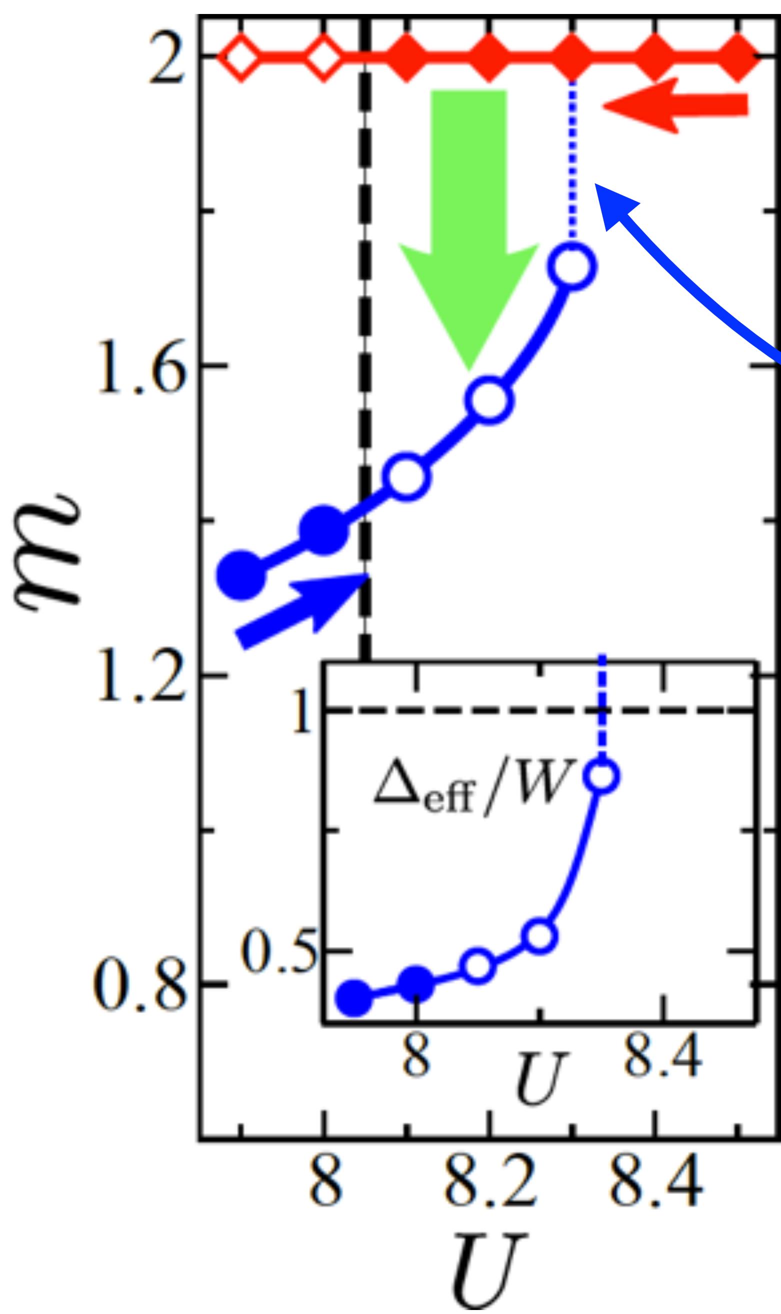
Goodenough's view of insulating VO_2



the transition is driven not just by opening a hybridisation gap between $d_{||}$ and $d_{||}^*$ orbitals as a result of dimerisation along the c-axis, but also, and maybe mostly, by the increase of crystal field splitting between $d_{||}$ and π^* orbitals.

state variable that better characterises the transition

m = (occupation band 1) - (occupation band 2)

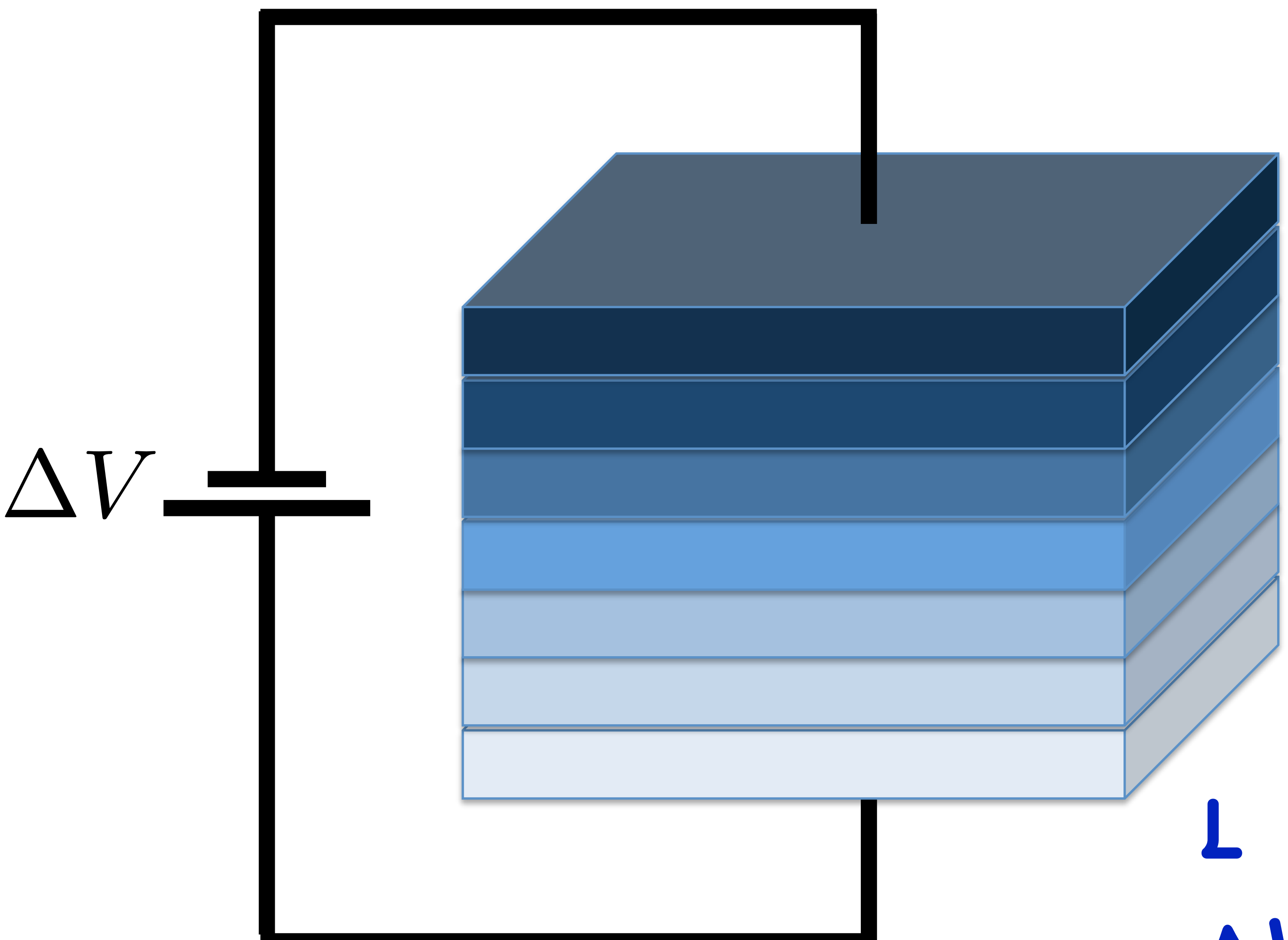


critical $U_{MIT} \approx 8.05$ of the 1st order Mott transition

spinodal point $U_s \approx 8.3$ above which the metal is not stable anymore

for $U_{MIT}<U<U_s$ there is coexistence between the stable insulator and a metastable metal

Geometry used to investigate the electric breakdown



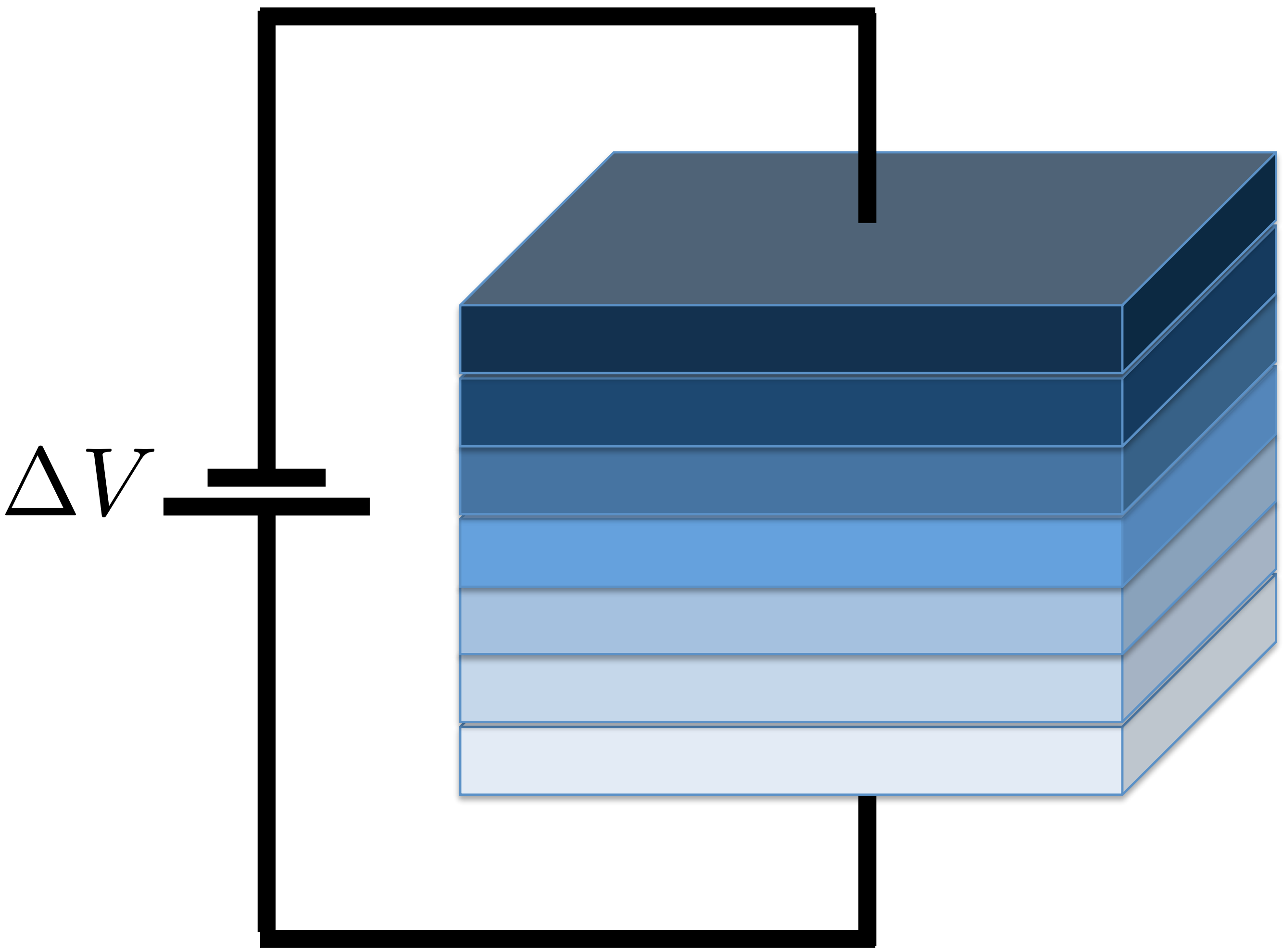
Open circuit mimicking a FET in a slab geometry

L = number of layers

$\Delta V/L$ = E (electric field)

Tool: inhomogeneous DMFT

Result: when $U>U_{MIT}$ for electric fields E above a threshold E_{th} the insulator turns into a conducting state

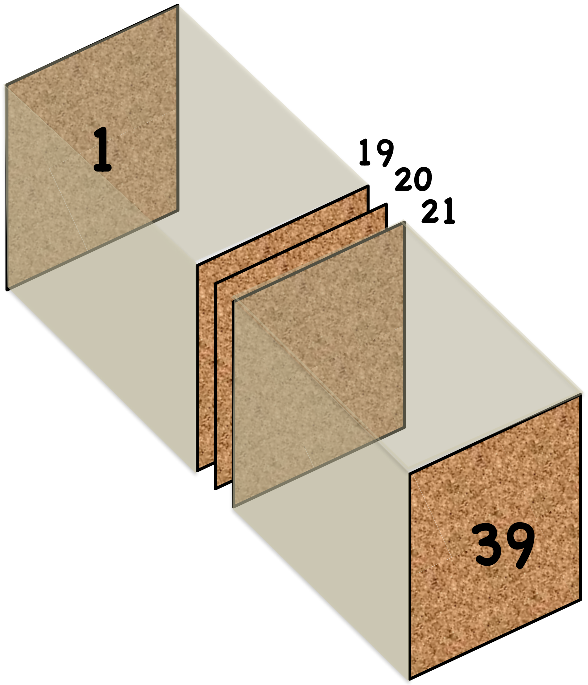


L = number of layers

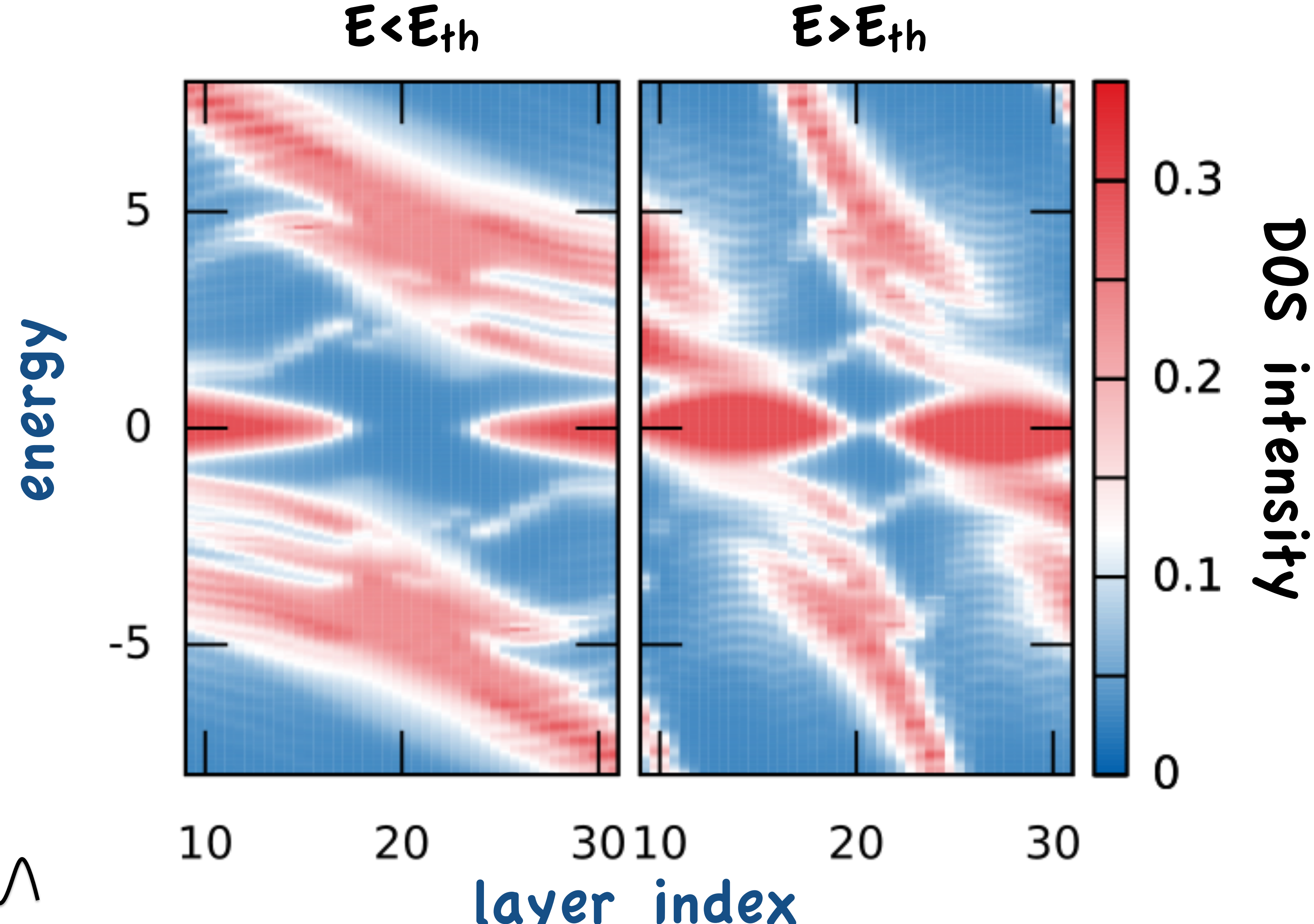
$\Delta V/L = E$ (electric field)

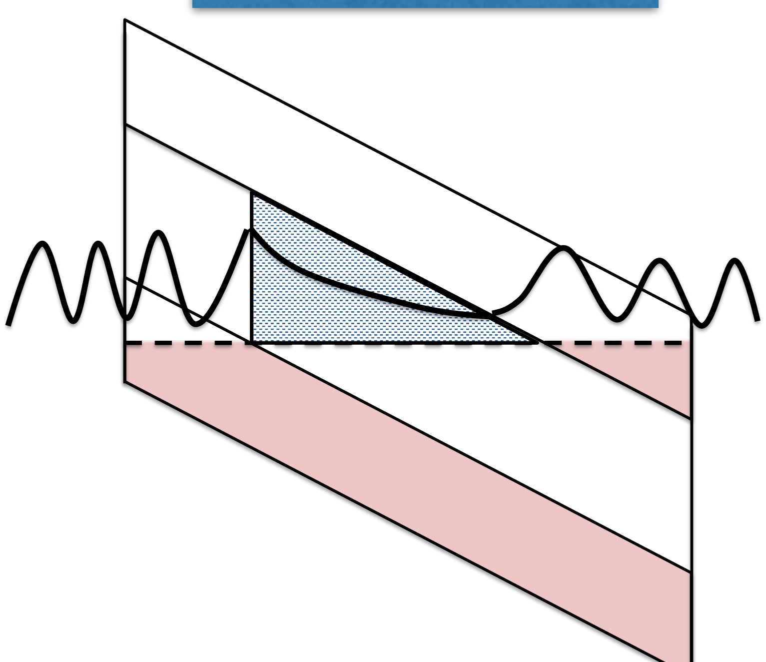
Is there any difference if the system is inside, $U_{MIT}<U<U_S$, or outside, $U>U_S$, insulator-metal coexistence?

Electric breakdown outside insulator-metal coexistence: $U=8.5>U_s$



layer dependent DOS

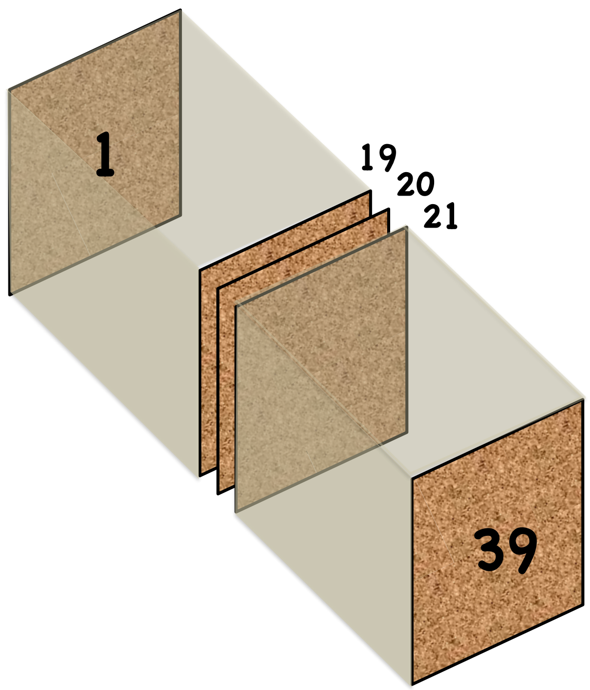


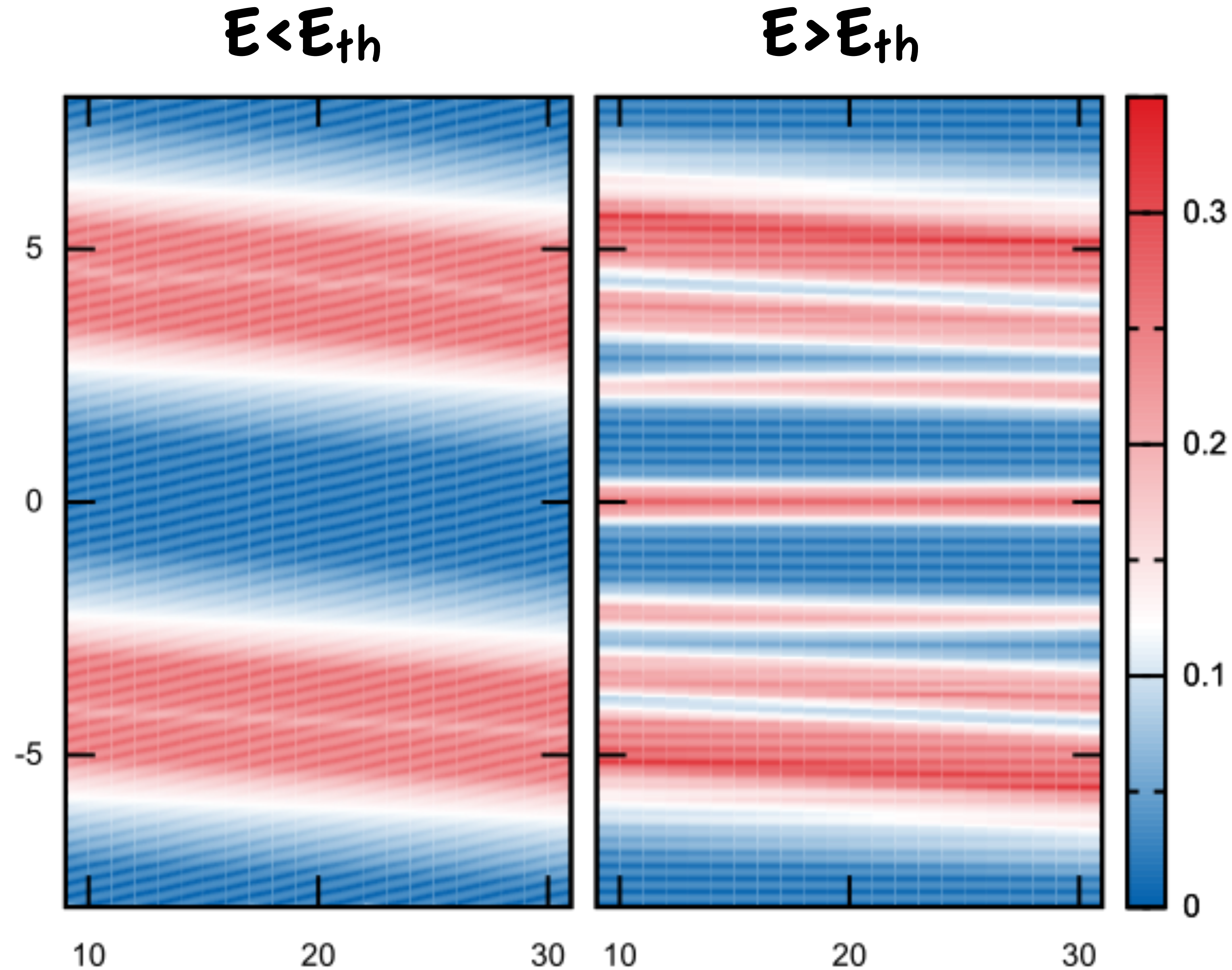


conventional Zener breakdown!

Electric breakdown inside insulator-metal coexistence:

$U_{MIT} < U = 8.1 < U_s$

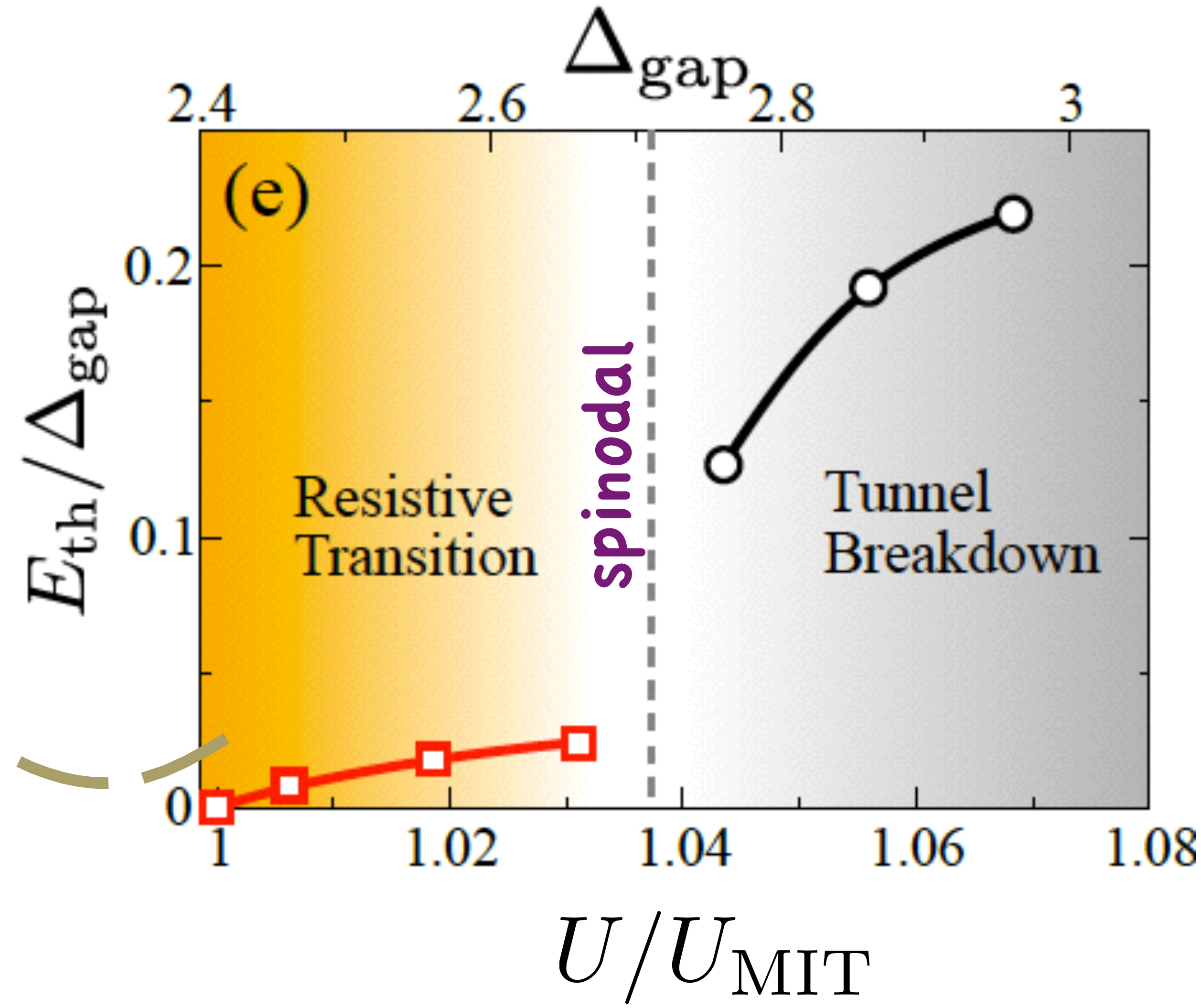




a genuine resistive transition: the insulator suddenly turns into quite a homogeneous metal

Strikingly different electric breakdown inside w.r.t. outside insulator-metal coexistence

threshold field E_{th} much smaller than the gap Δ_{GAP}! **WHY?**

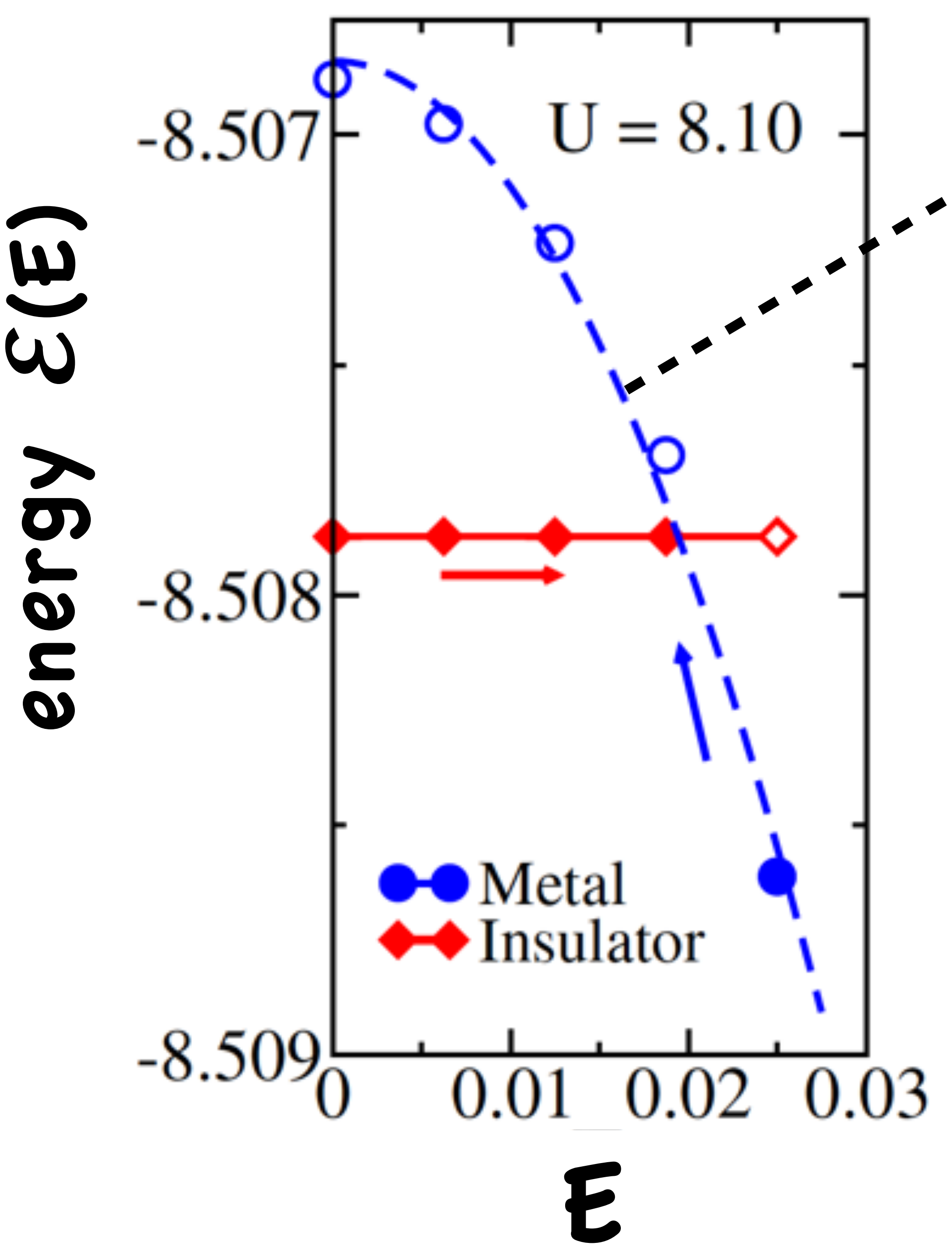


E_{th} changes sizeably crossing the spinodal point, though the equilibrium gap Δ_{GAP} varies imperceptibly! **WHY?**

the metal stabilised by E is adiabatically connected to the metastable metal at E=0!

$$\mathcal{E}(E) \simeq \mathcal{E}(0) - \frac{1}{2}\,\Pi\,E^2$$

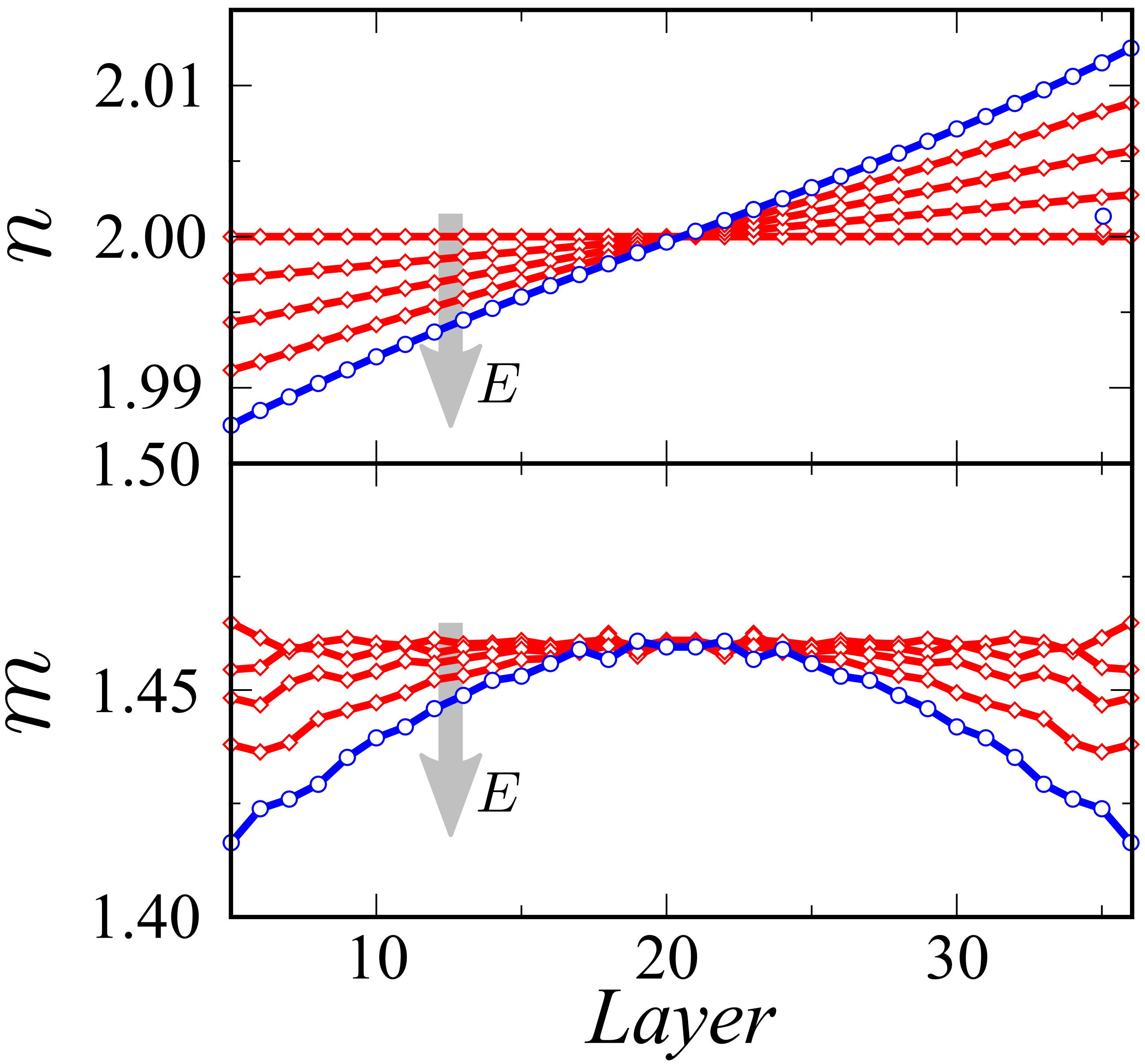
polarisability



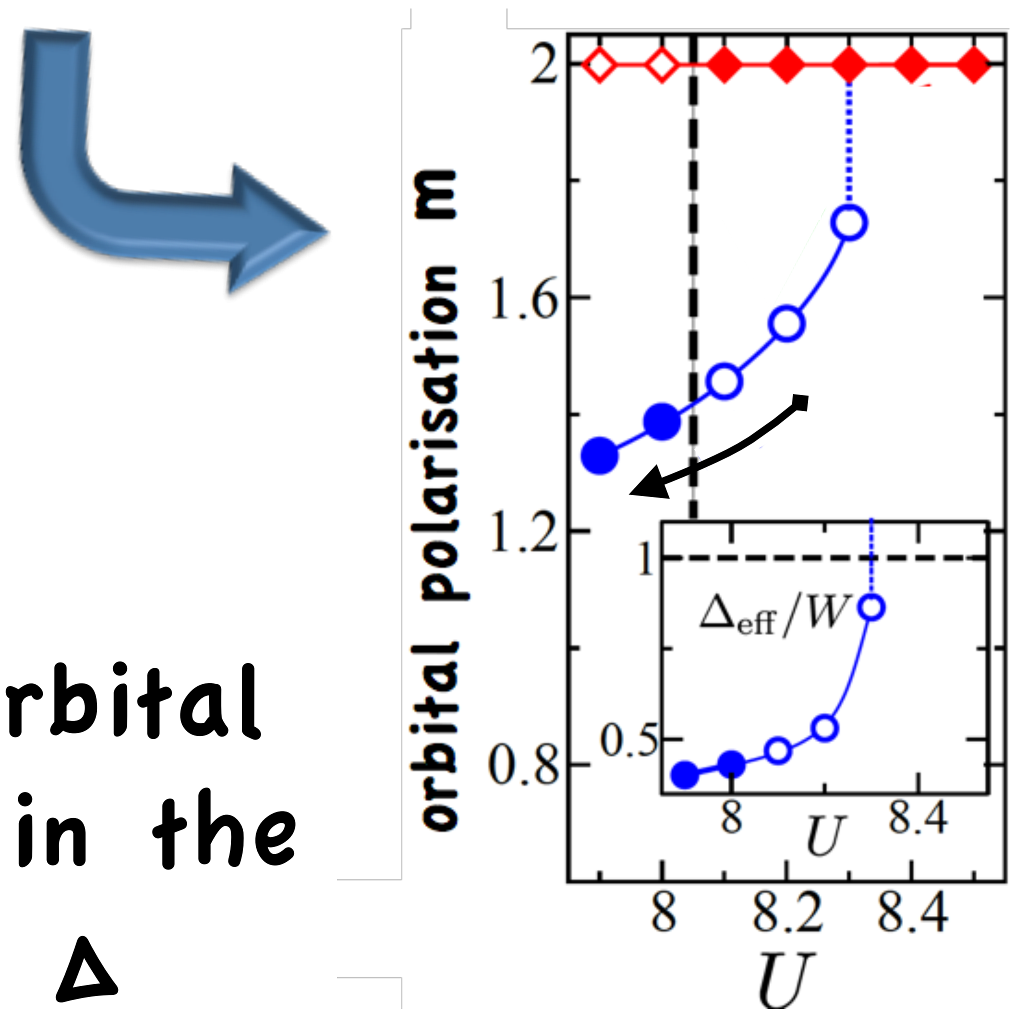
the energy of the polarisable metal is lowered by E and eventually crosses that of the incompressible insulator

the transition occurs when the metal is still in the linear response regime — no critical issue about non-equilibrium effects!

the metallic character is strengthened by the field

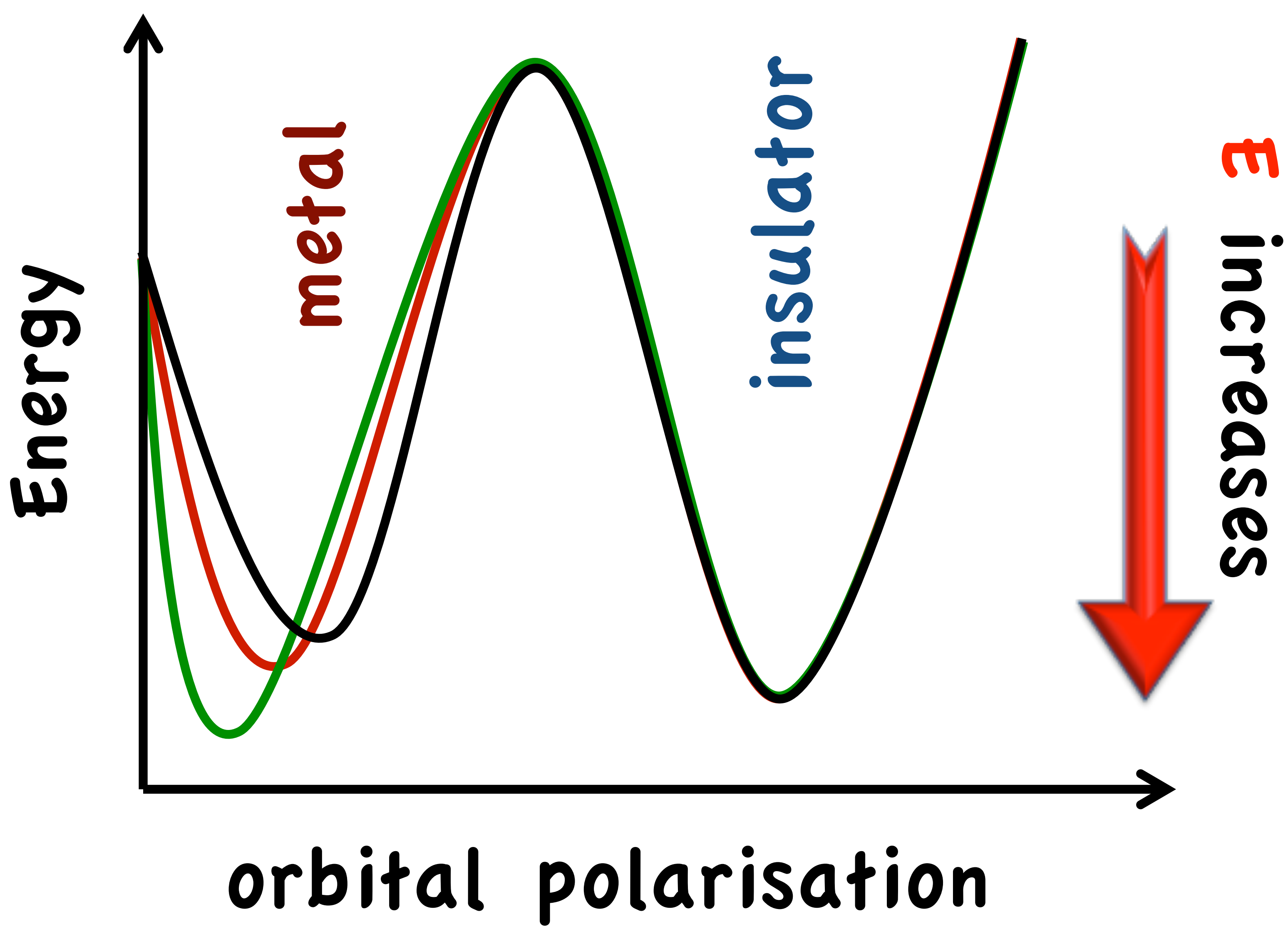


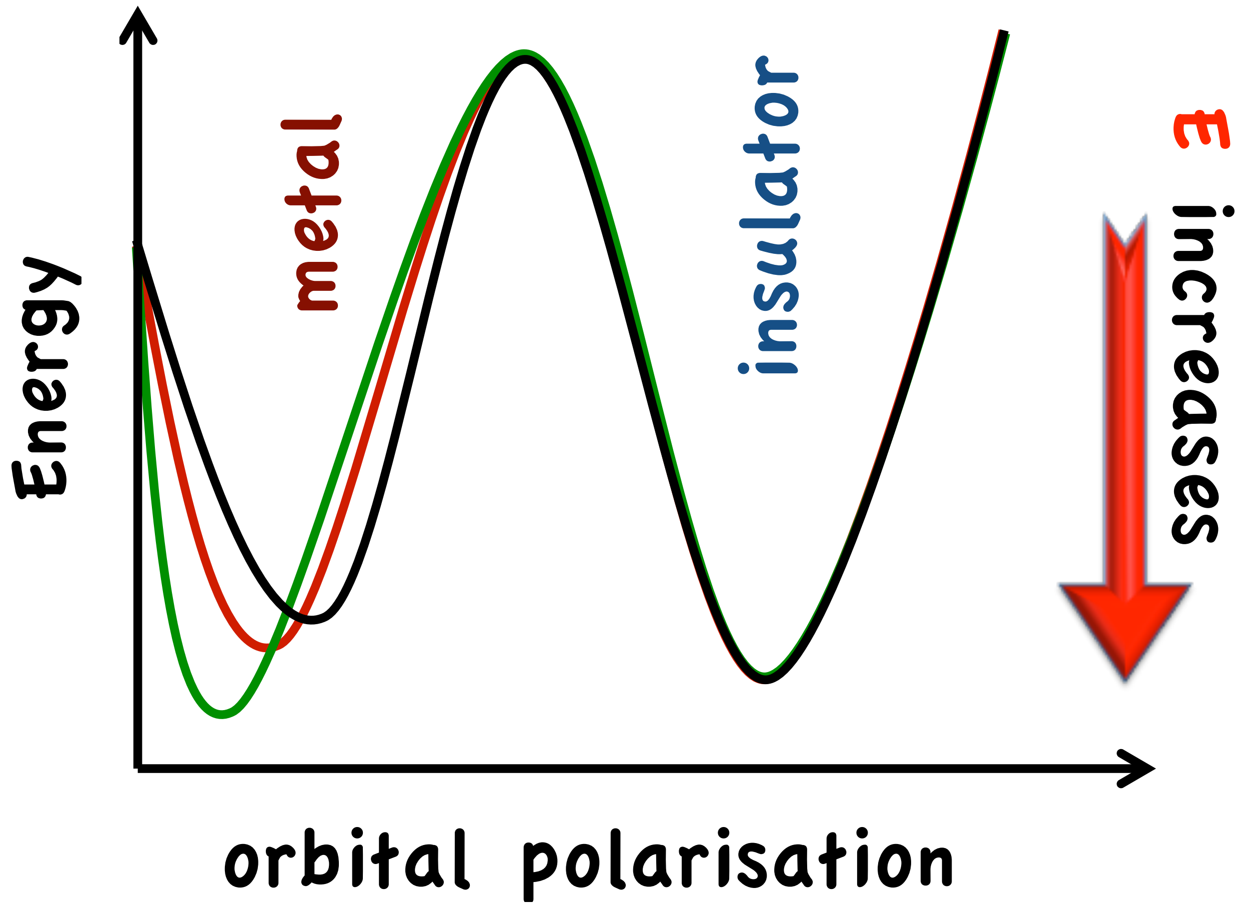
Δm > |Δn|, contrary to the naïve expectation that doped electrons on the right side occupy orbital 2, and doped holes on the left side are taken out of orbital 1



the electric field lowers the orbital polarisation effectively moving in the phase space as if U and/or Δ diminished

In summary: the electric field lowers the energy of the formerly metastable metal, until it eventually crosses the energy of the insulator





a remark: in our model the resistive transition seems to occur abruptly, without being preceded by the appearance of metal wetting layers at the opposite sides of the slab, though the potential is bigger at the surfaces.

We don't exactly understand why we do not observe wetting (a wetting interface too expensive in our finite size slab?), as well as we still don't know what would happen should we include long range Coulomb and dispersion forces.

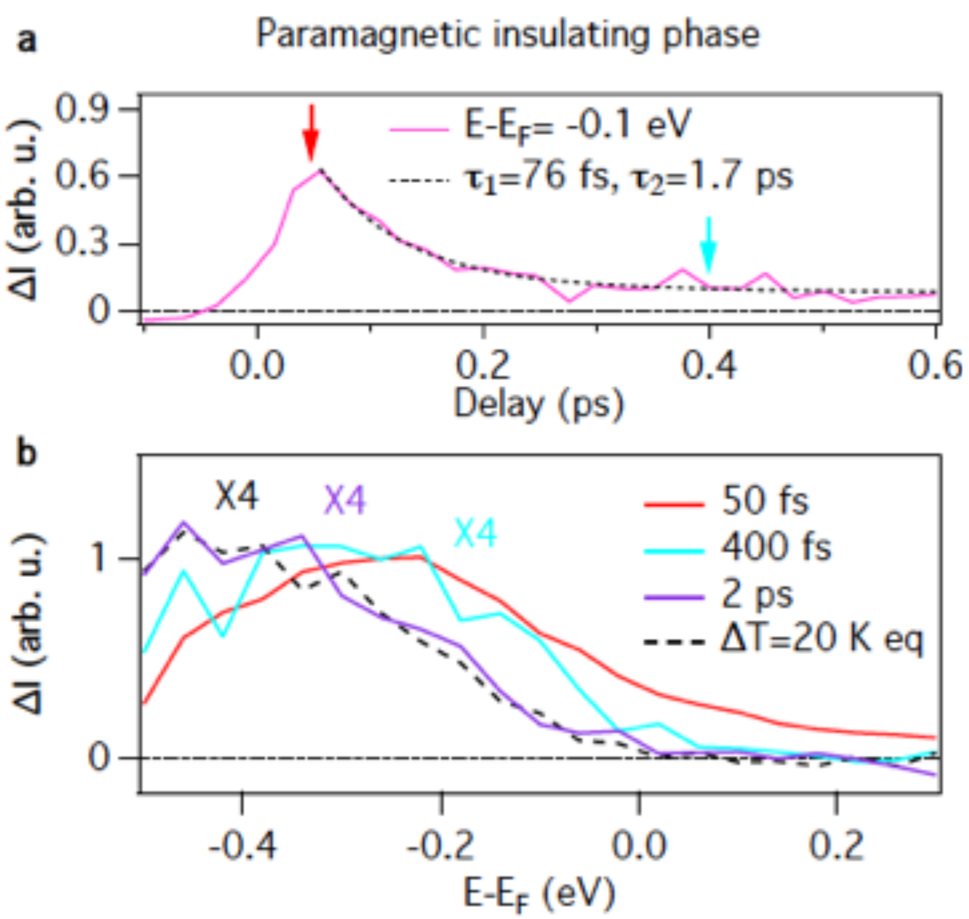
Preliminary conclusion: the electric field is able to stabilise the more polarisable, formerly metastable, metal within the insulator-metal coexistence domain

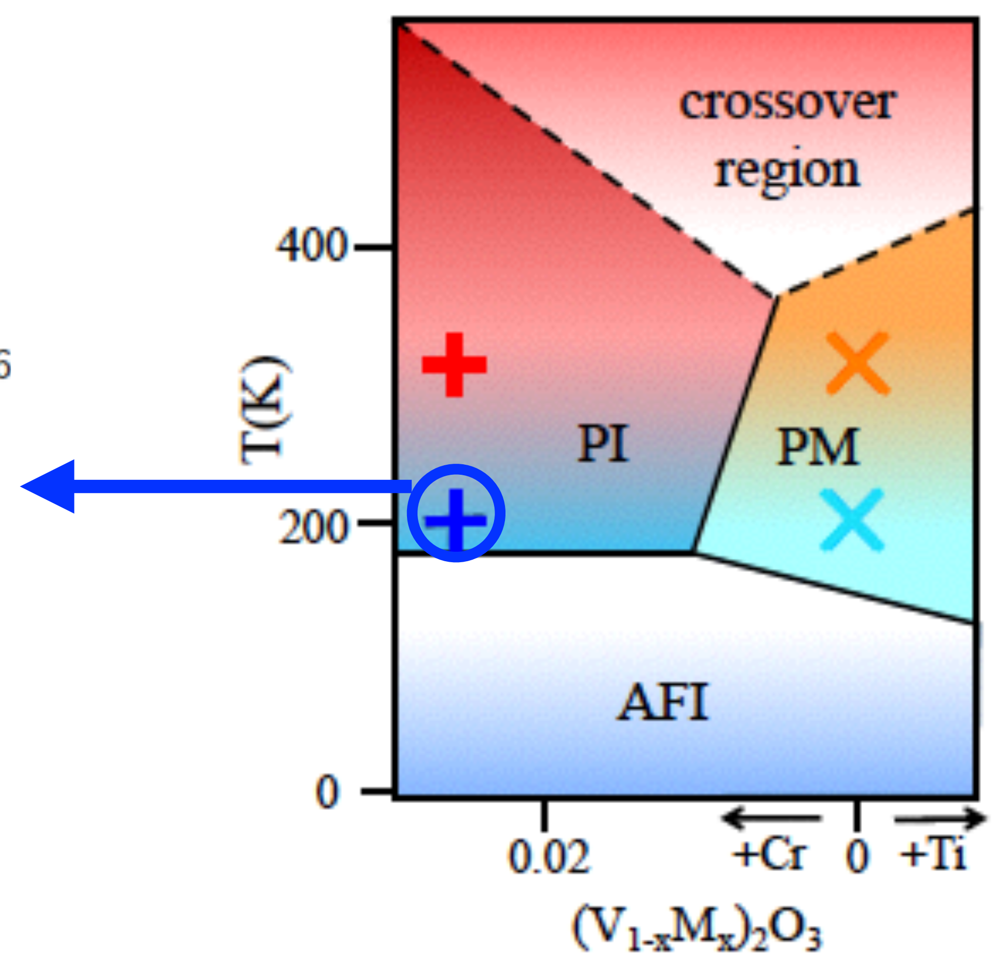
Any other interesting phenomena that may appear near a 1^{st} order Mott transition?

G. Lantz's talk this morning ...

Ultrafast evolution and transient phases of a prototype out-of-equilibrium Mott-Hubbard material

G. Lantz,[1,2] B. Mansart,[1] D. Grieger,[3] D. Boschetto,[4] N. Nilforoushan,[1] E. Papalazarou,[1] N. Moisan,[1] L. Perfetti,[5] V. L. R. Jacques,[1] D. Le Bolloch,[1] C. Laulhé,[6,7] S. Ravy,[6,1] J.-P. Rueff,[6] T.E. Glover,[8] M.P. Hertlein,[8] Z. Hussain,[8] S. Song,[9] M. Chollet,[9] M. Fabrizio,[3] and M. Marsi[1]



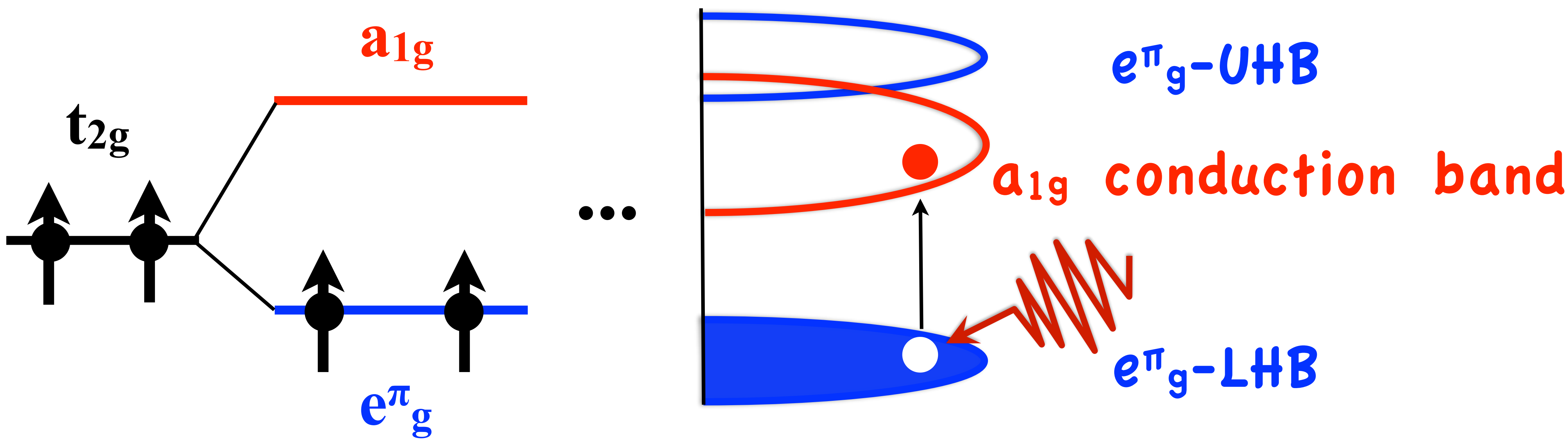


V_2O_3

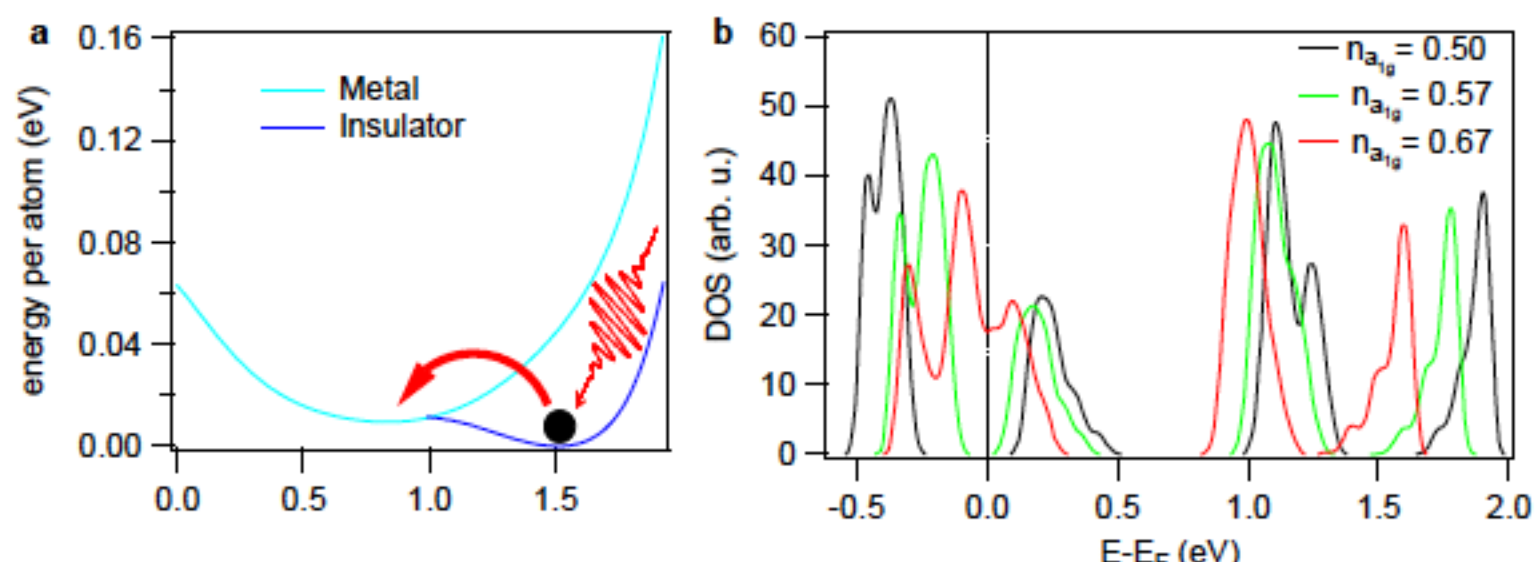
the gap transiently collapses!

the system thermalises only after ~ 2 ps

theoretical explanation



Hartree-Fock
with realistic
tight-binding
parameters

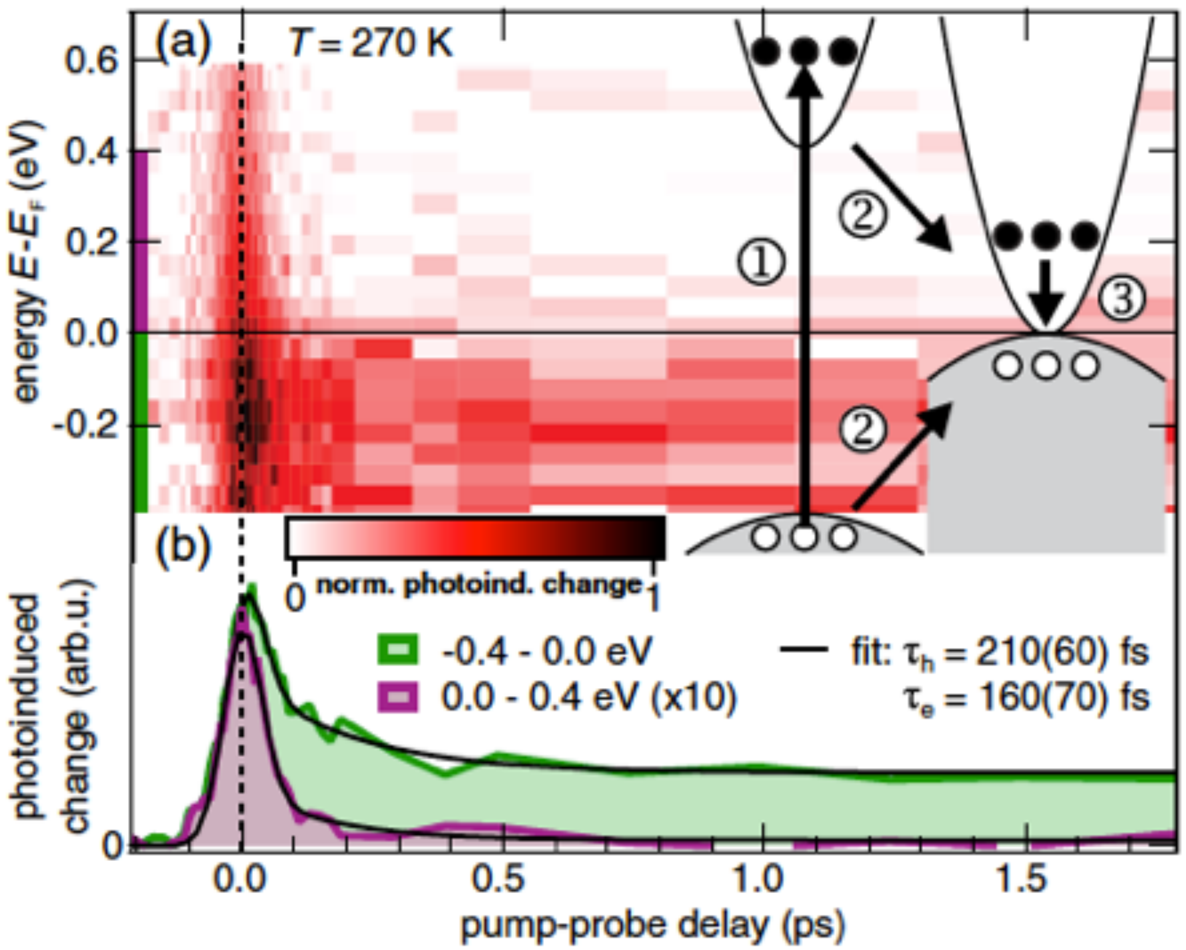


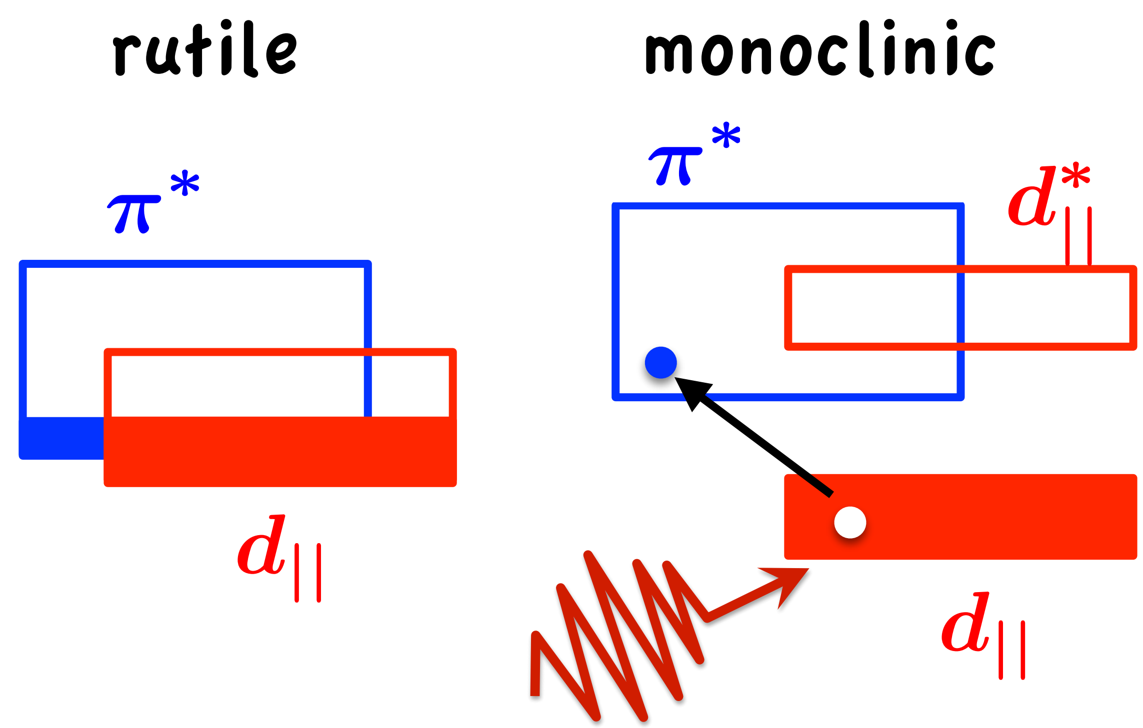
$$m = n(e^{\pi}_{g}) - n(a_{1g})$$

different physics, yet the same mechanism

Instantaneous Band Gap Collapse in Photoexcited Monoclinic VO_2 due to Photocarrier Doping

Daniel Wegkamp,[1] Marc Herzog,[1] Lede Xian,[2,3] Matteo Gatti,[4,3,5] Pierluigi Cudazzo,[2,3] Christina L. McGahan,[6] Robert E. Marvel,[6] Richard F. Haglund, Jr.,[6] Angel Rubio,[2,7,3,1] Martin Wolf,[1] and Julia Stähler[1,*]





the laser pulse transfers electrons from the occupied $d_{||}$ band to the empty π^* band;

it effectively couples to the state variable

$$m = n(d_{||}) - n(\pi^*)$$

… and still more

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Ultrafast Switching to a Stable Hidden Quantum State in an Electronic Crystal

L. Stojchevska,[1,2] I. Vaskivskyi,[1] T. Mertelj,[1] P. Kusar,[1] D. Svetin,[1] S. Brazovskii,[3,4] D. Mihailovic[1,2,5*]

Hidden states of matter may be created if a system out of equilibrium follows a trajectory to a state that is inaccessible or does not exist under normal equilibrium conditions. We found such a hidden (H) electronic state in a layered dichalcogenide crystal of *1T*-TaS_2 (the trigonal phase of tantalum disulfide) reached as a result of a quench caused by a single 35-femtosecond laser pulse. In comparison to other states of the system, the H state exhibits a large drop of electrical resistance, strongly modified single-particle and collective-mode spectra, and a marked change of optical reflectivity. The H state is stable until a laser pulse, electrical current, or thermal erase procedure is applied, causing it to revert to the thermodynamic ground state.

RESEARCH ARTICLE

MATERIALS SCIENCE

Memristive phase switching in two-dimensional 1T-TaS_2 crystals

10.1126/sciadv.1500606

Masaro Yoshida,[1*] Ryuji Suzuki,[1] Yijin Zhang,[1] Masaki Nakano,[1] Yoshihiro Iwasa[1,2]

Scaling down materials to an atomic-layer level produces rich physical and chemical properties as exemplified in various two-dimensional (2D) crystals including graphene, transition metal dichalcogenides, and black phosphorus. This is caused by the dramatic modification of electronic band structures. In such reduced dimensions, the electron correlation effects are also expected to be significantly changed from bulk systems. However, there are few attempts to realize novel phenomena in correlated 2D crystals. We report memristive phase switching in nano-thick crystals of 1T-type tantalum disulfide (1T-TaS_2), a first-order phase transition system. The ordering kinetics of the phase transition were found to become extremely slow as the thickness is reduced, resulting in an emergence of metastable states. Furthermore, we realized unprecedented memristive switching to multistep nonvolatile states by applying an in-plane electric field. The reduction of thickness is essential to achieve such nonvolatile electrical switching behavior. The thinning-induced slow kinetics possibly make the various metastable states robust and consequently realize the nonvolatile memory operation. The present result indicates that a 2D crystal with correlated electrons is a novel nano-system to explore and functionalize multiple metastable states that are inaccessible in its bulk form.

Yoshida *et al.* Sci. Adv. 2015;1:e1500606 2 October 2015

Conclusions: the importance of being inside … … insulator-metal coexistence

- In narrow gap Mott insulators the proximity to the first order Mott transition entails several interesting phenomena
  - ✓ field-driven non-Zener resistive transition
  - ✓ light-induced gap-collapse
  - ✓ wetting at interfaces
  - ✓ new non-thermal hidden phases

Thank you!