

Universal dielectric breakdown and synaptic behaviour in Mott insulators

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R. Weht



Refs:

V. Guiot et al, Nat Comm (2013)

P. Stoliar et al., Adv. Mat. (2013)

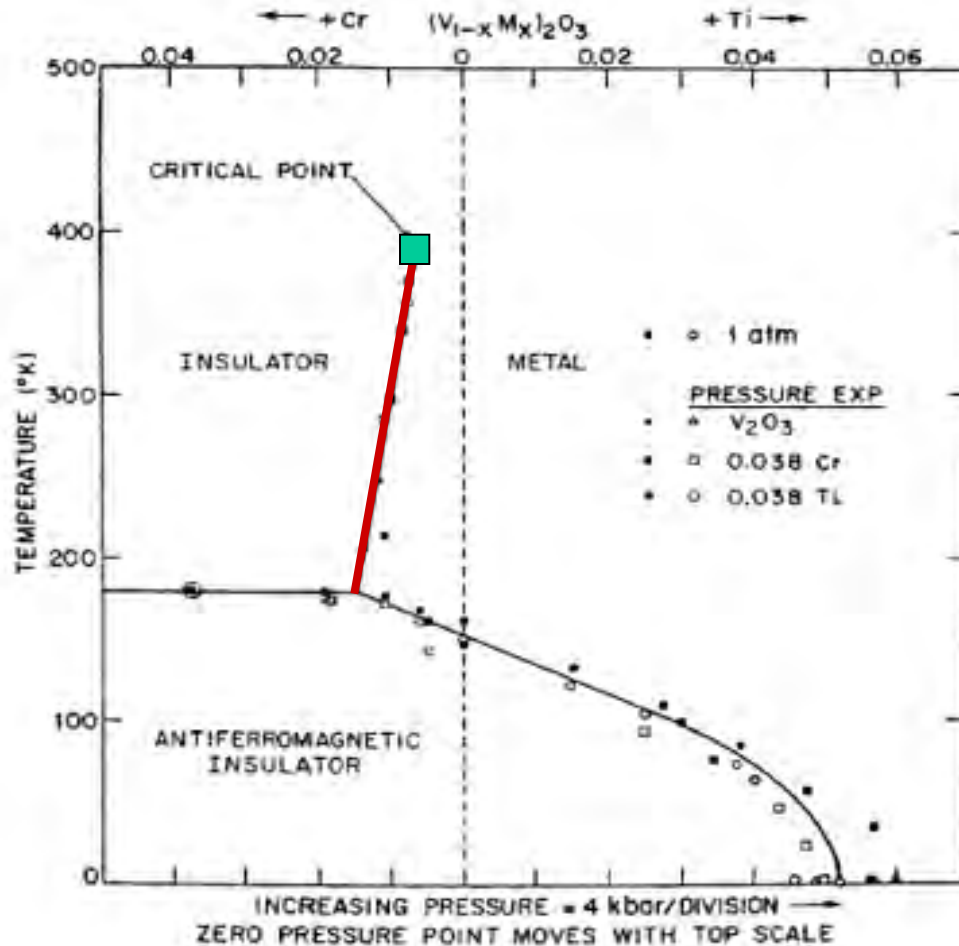
A. Camjayi et al., Phys Rev Lett (2014)

L. Cario et al Adv Func Mat (in press) **Review**

What is a Mott transition?

The classic example: Mott transition in V_2O_3

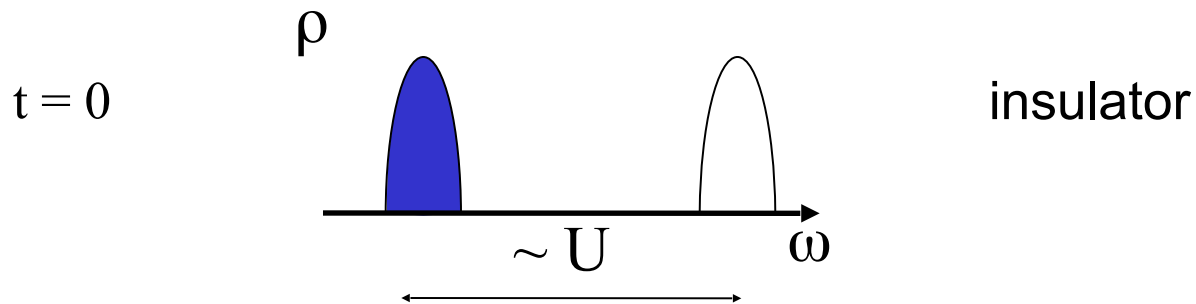
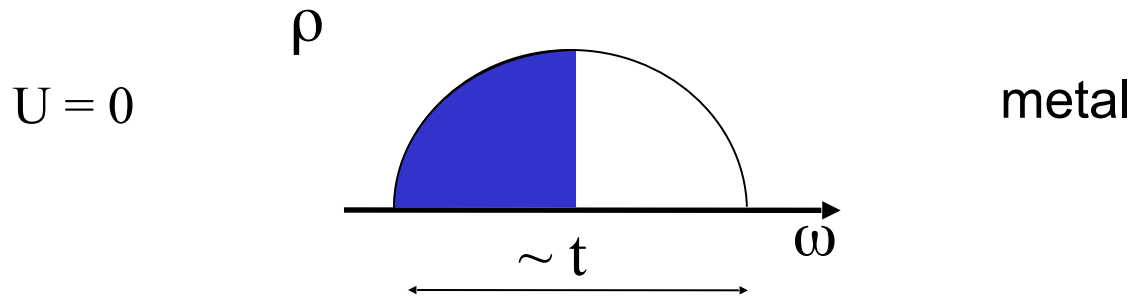
T



pressure or chemical substitution

The Hubbard model is a minimal model for the metal – insulator transition

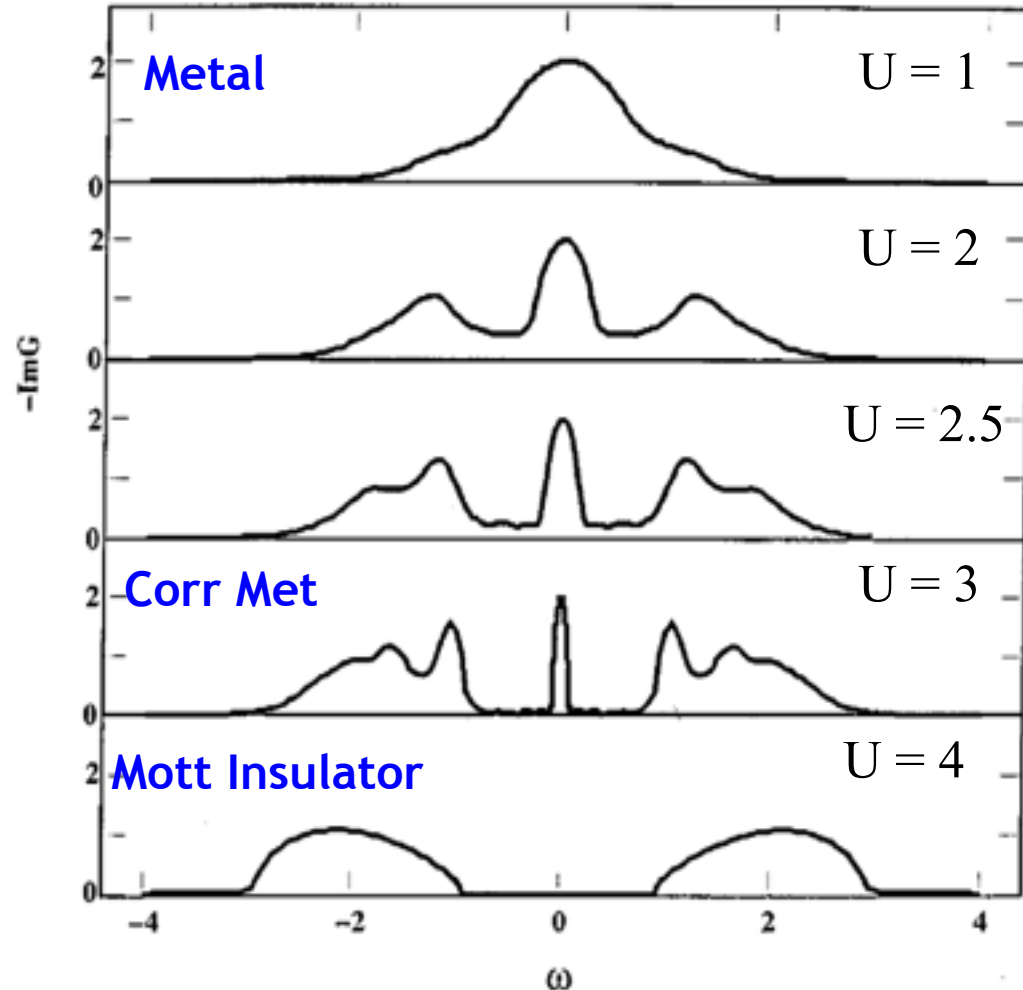
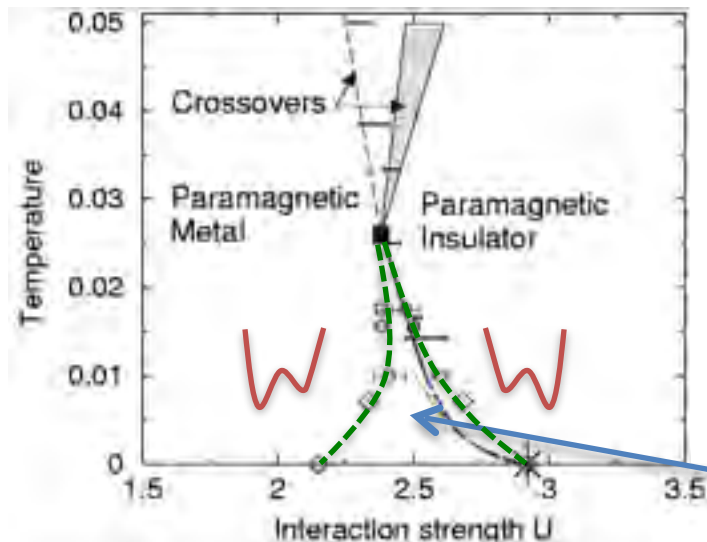
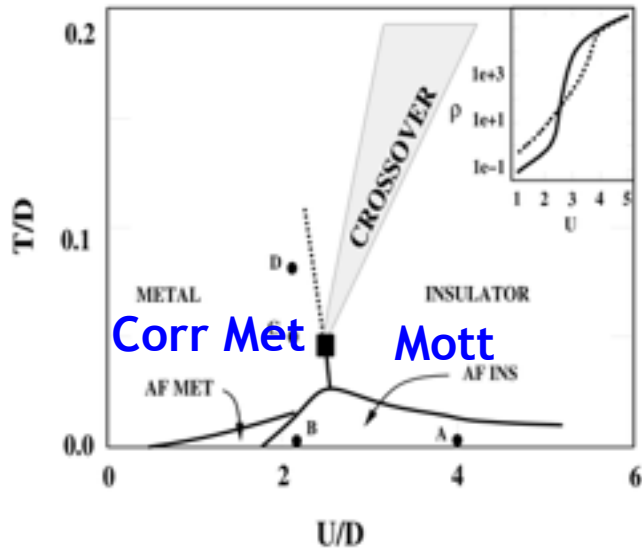
$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



DMFT of the Mott - Hubbard transition

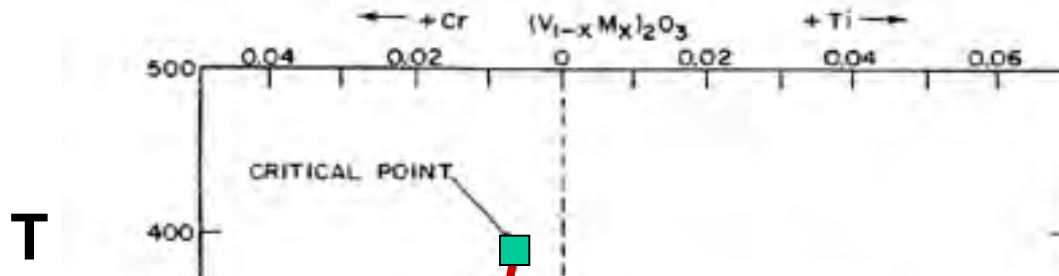
A. Georges et al. RMP '96

XY Zhang, MR, G. Kotliar PRL '92



Coexistence region: 2 solutions

The classic example: Mott transition in V_2O_3



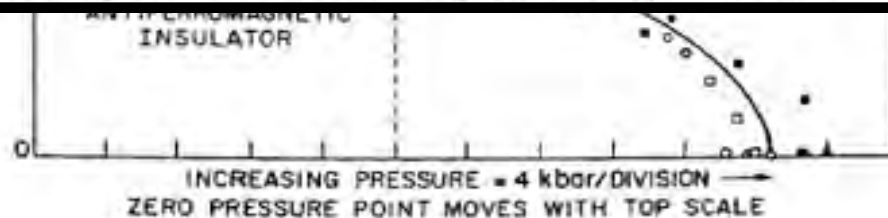
Phys. Status Solidi B 250, No. 7, 1251–1264 (2013) / DOI 10.1002/pssb.201248476

physica **p** status **s** solidi **s**^b
www.pss-b.com
basic solid state physics

Mott–Hubbard transition in V_2O_3 revisited

Feature Article

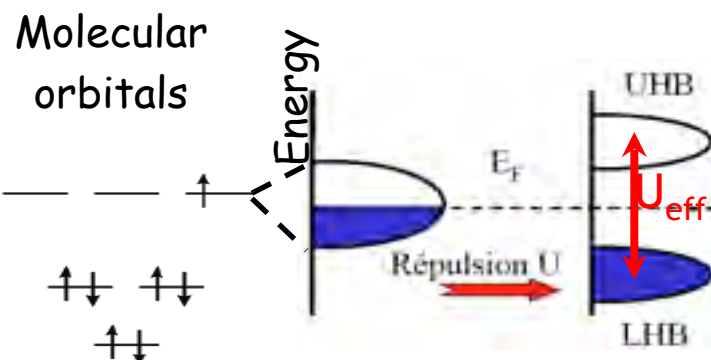
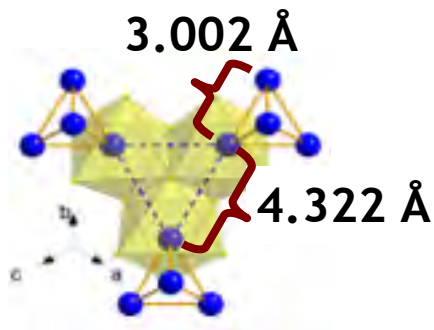
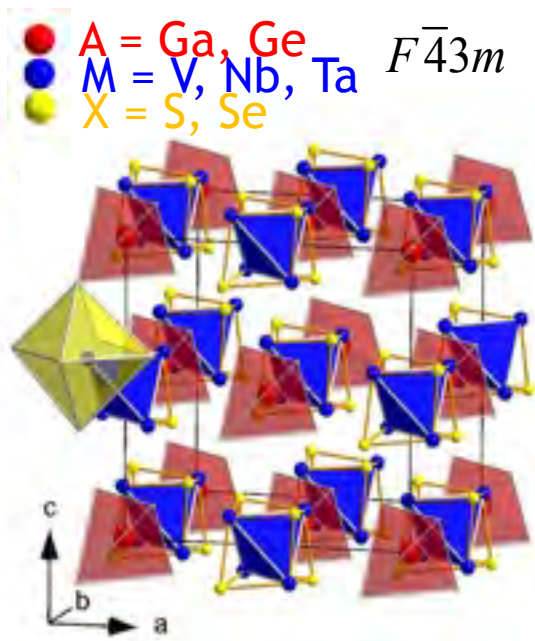
P. Hansmann^{1,2}, A. Toschi¹, G. Sangiovanni^{1,3}, T. Saha-Dasgupta⁴, S. Lupi⁵, M. Marsi⁶



pressure or chemical substitution

Do Mott - Hubbard systems exist in Nature?

AM_4X_8 family: tailor-made 3D Mott systems

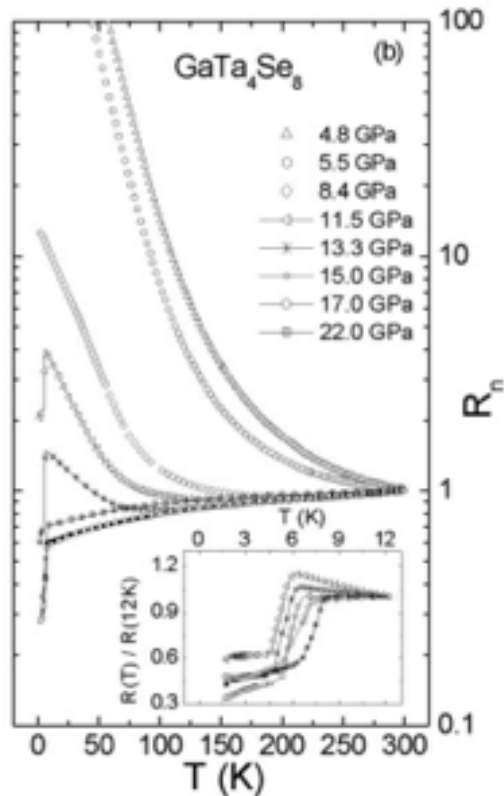


Gap ~ 0.20 eV

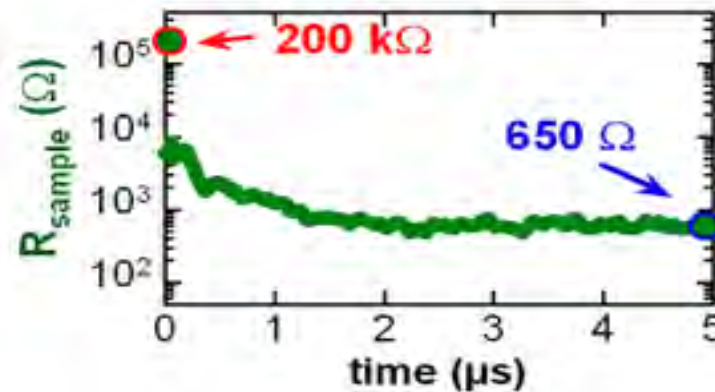
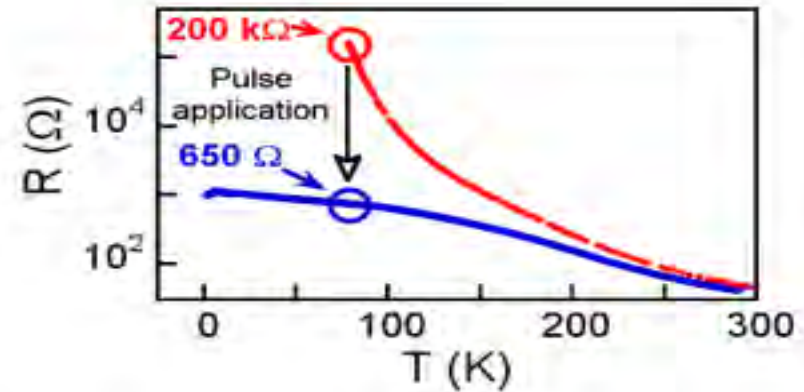
Pocha, R. et al., *J. Am. Chem. Soc.* 127, 8732 (2005)

Metal - Insulator transition in GTS

Pressure driven Mott transition



E-field driven Mott transition



Abd-Elmeguid et al., PRL '04

Non Volatile Resistive Switching, $t < 100$ ns

C. Vaju et al., Adv. Mater. '08

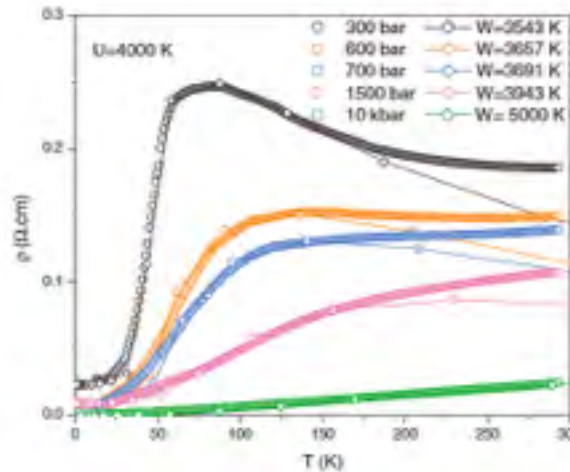
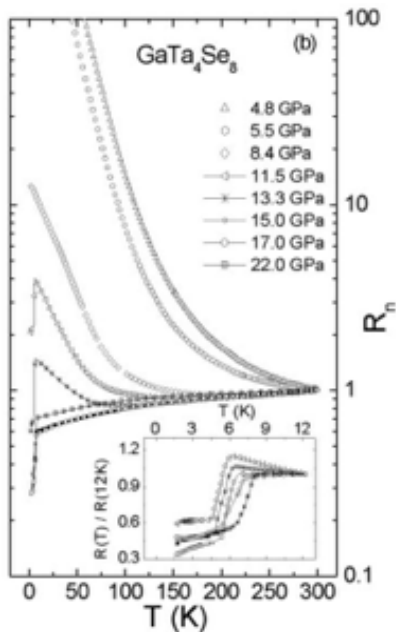
Is GaTa_4Se_8 (GTS) really a Mott-Hubbard system?

« Ideal system »

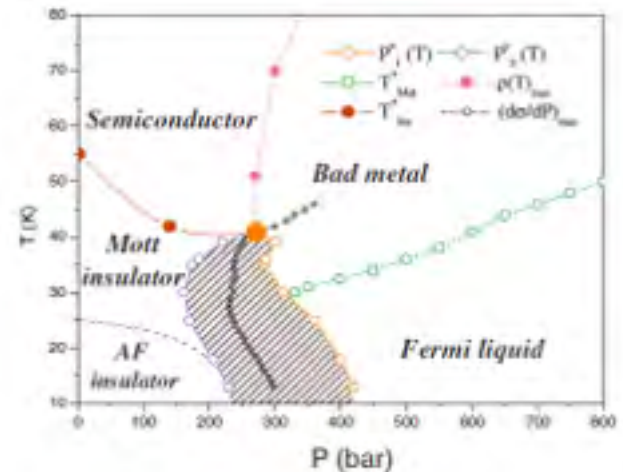
- 1 electron per Ta_4 cluster
- 3D fcc lattice
- Paramagnetic
- LDA predicts a metal

But does not match some DMFT key predictions

- No hysteresis
- $\rho(T)$ does not have non-monotonic behavior

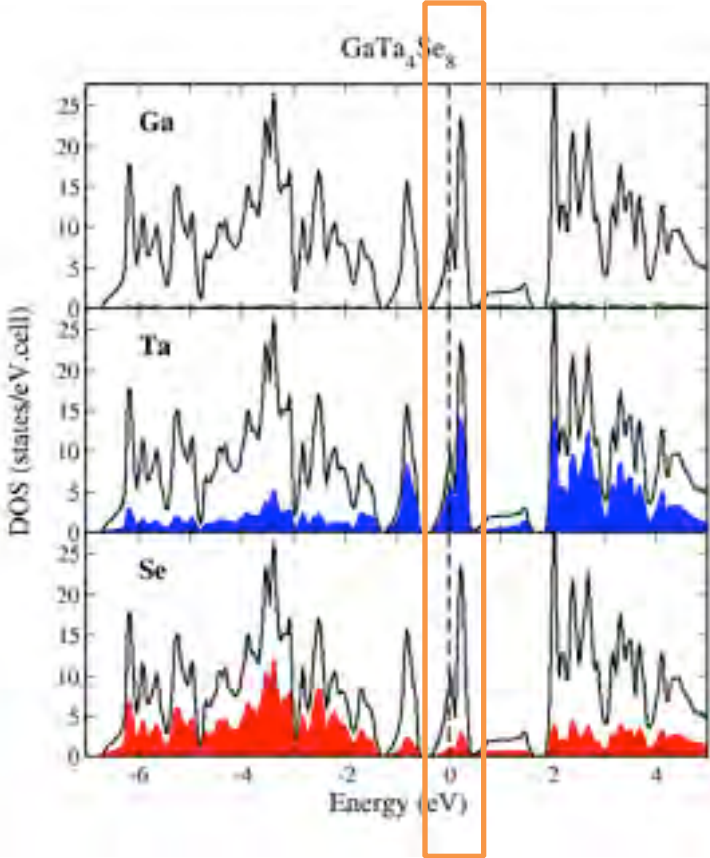
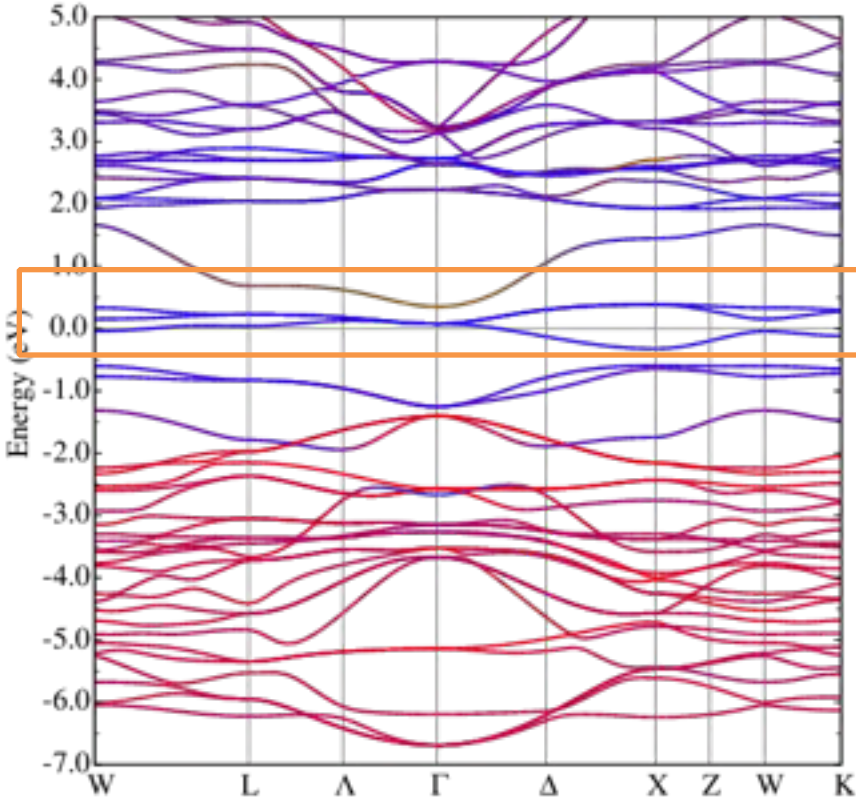


K-organics

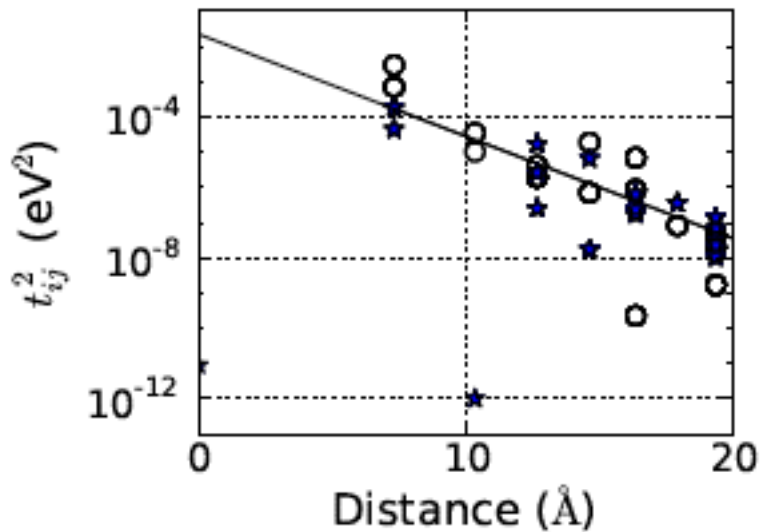
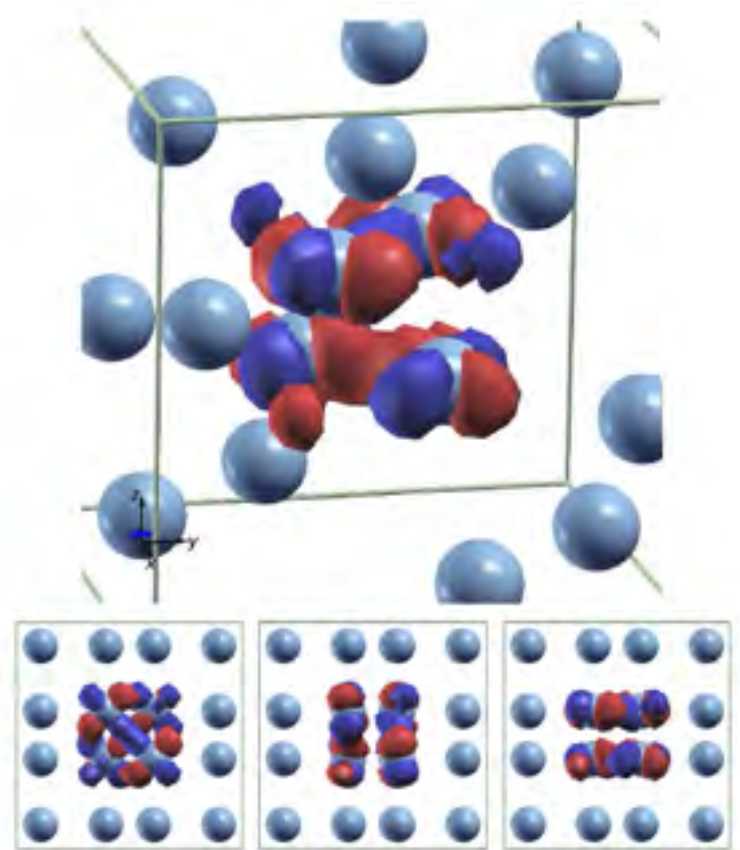
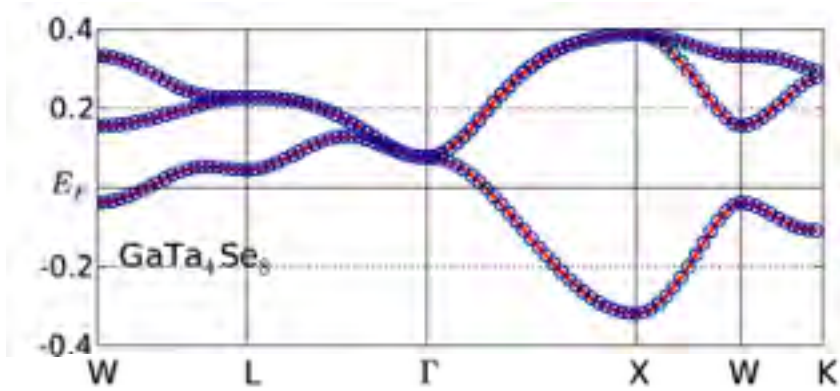


Limelette PRL (2003)

Conduction bands are isolated and have pure Ta character
Nice system for an LDA+DMFT study



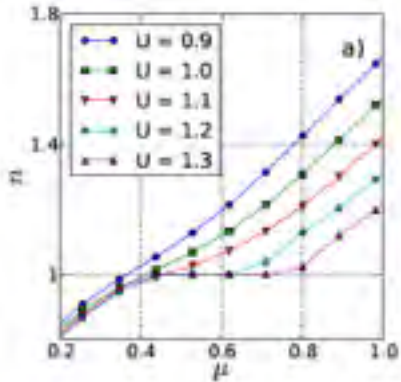
Wannier maximally localized molecular orbitals for Ta₄ tetrahedra



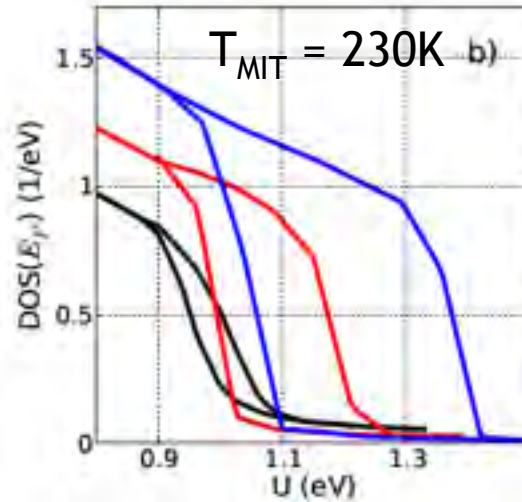
Cubic FCC structure, t_{2g} symmetry

What is U?

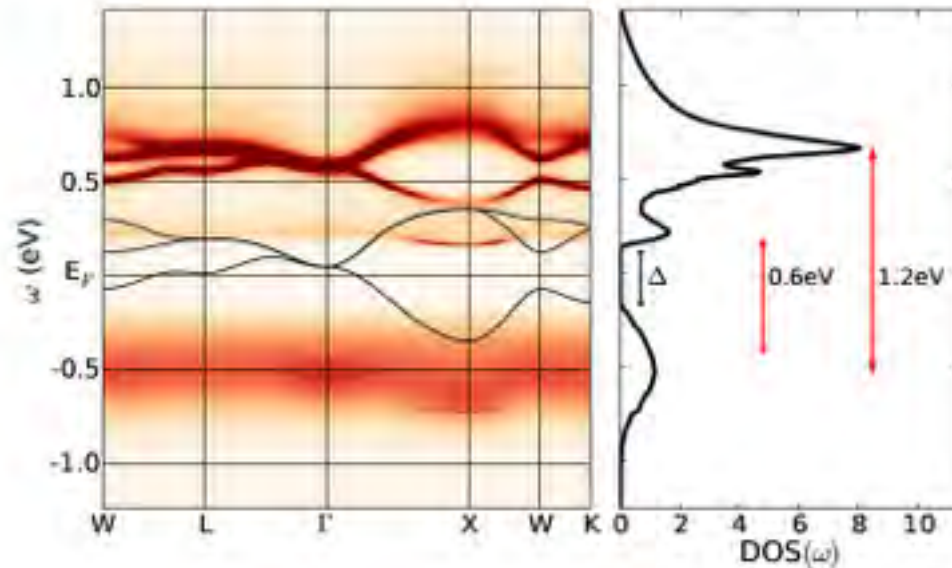
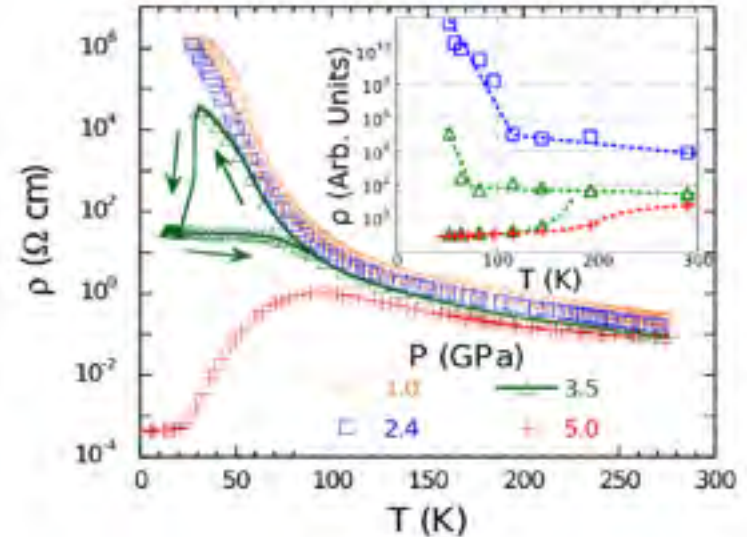
$U_c = 1.2 \text{ eV}$



hysteresis



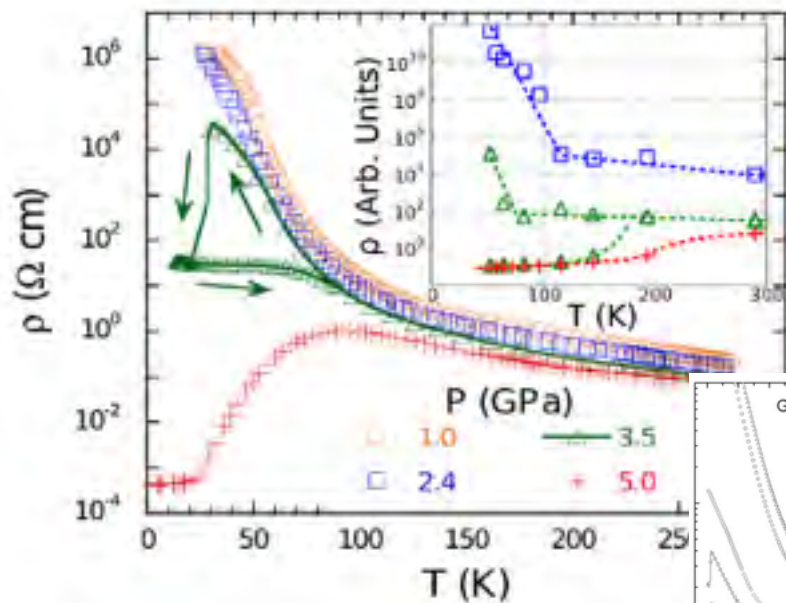
resistivity



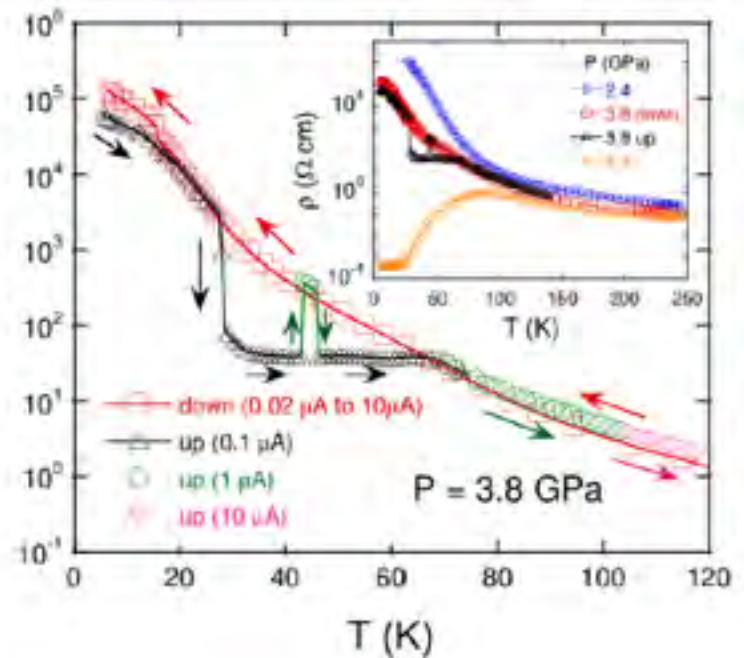
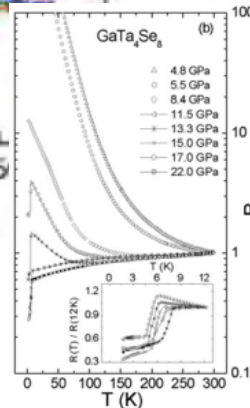
- 1st order transition T
- Optical conductivity
- Resistivity (activation gap)



Resistivity is nonmonotonic in the metal and has hysteresis at the IMT



single x-tal!



A. Camjayi et al., Phys Rev Lett (2014)

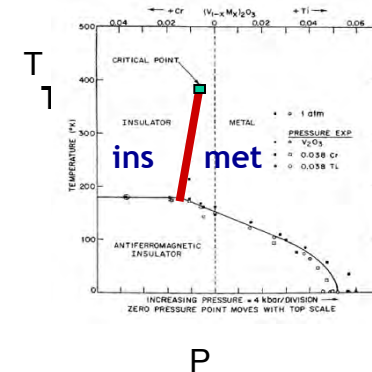
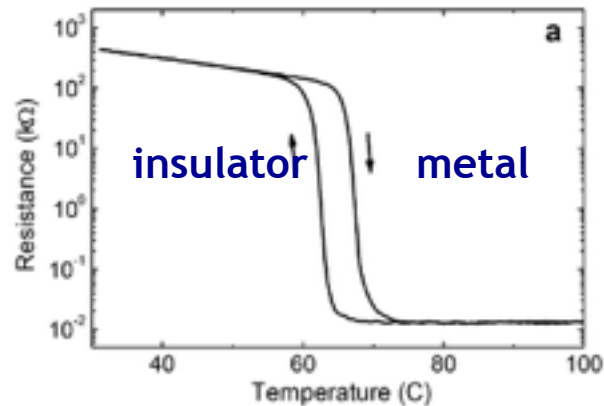
Abd-Elmeguid et al., PRL '04

Mott physics + electronics
« Mottronics »

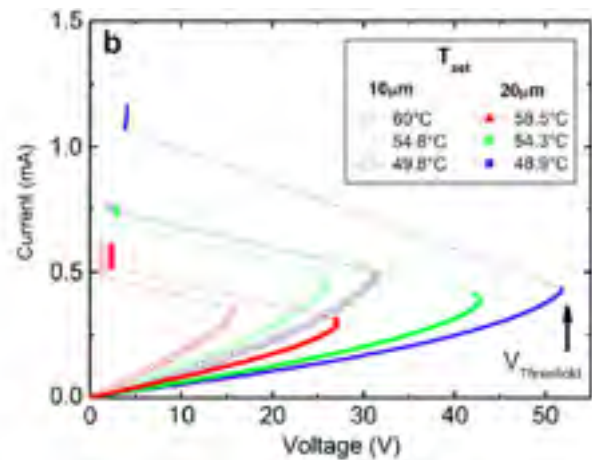
Applying strong E-fields to
Mott systems

Do not mix up with the Mott transition in VO_2

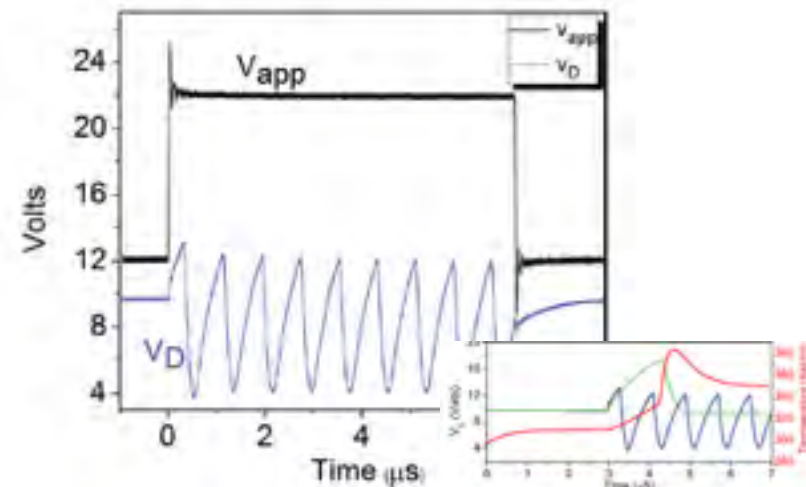
1st order transition driven by T



Joule heating effect

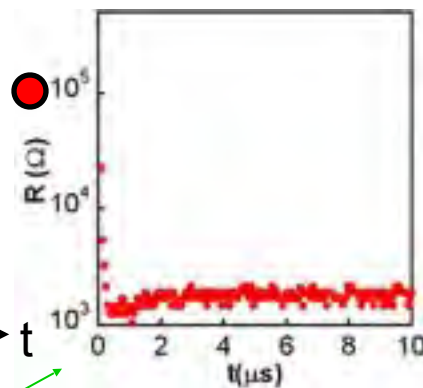
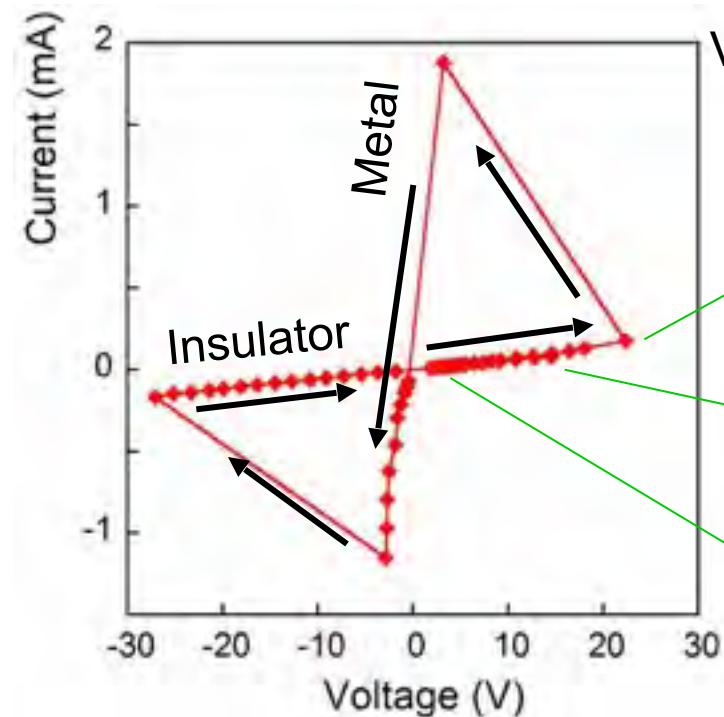


E-field effect



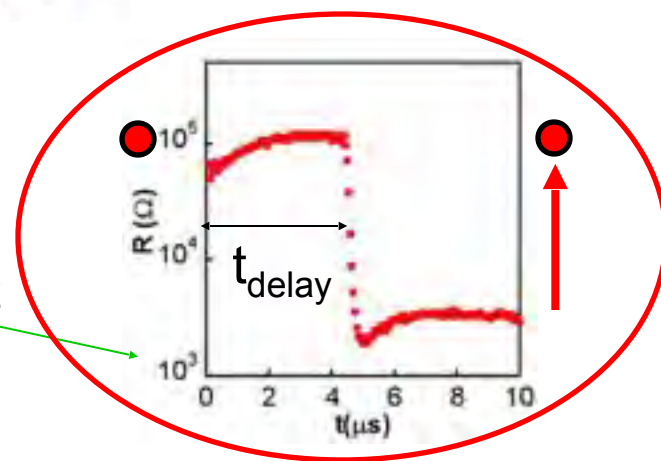
Three different regimes

GaTa₄Se₈ 77 K



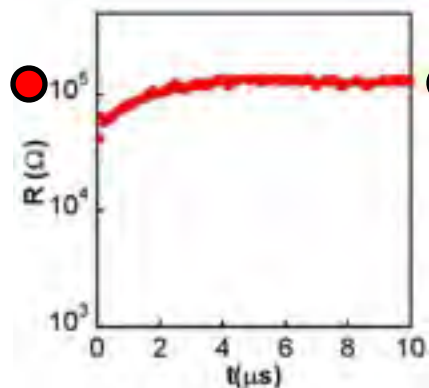
non-volatile RS

volatile RS

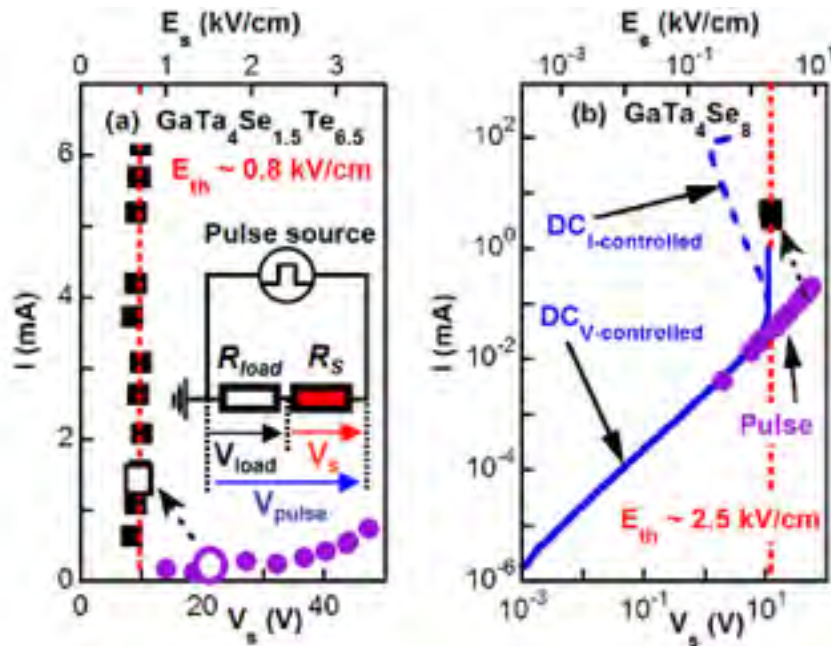
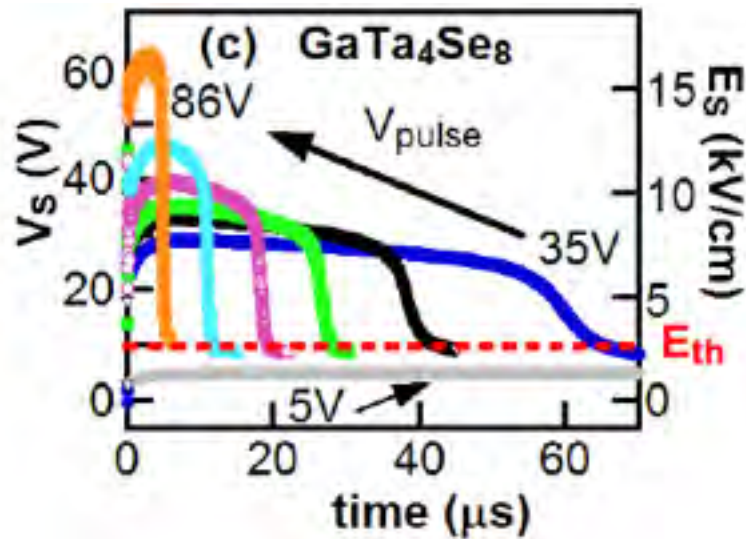


R_{bef}

R_{after}



E-field driven Mott transition in GTS



E-field threshold

Is the Mott electric-breakdown universal?

Three different Mott-insulators:

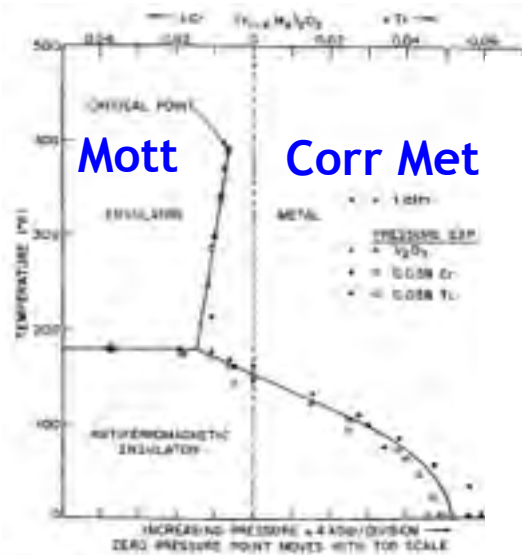
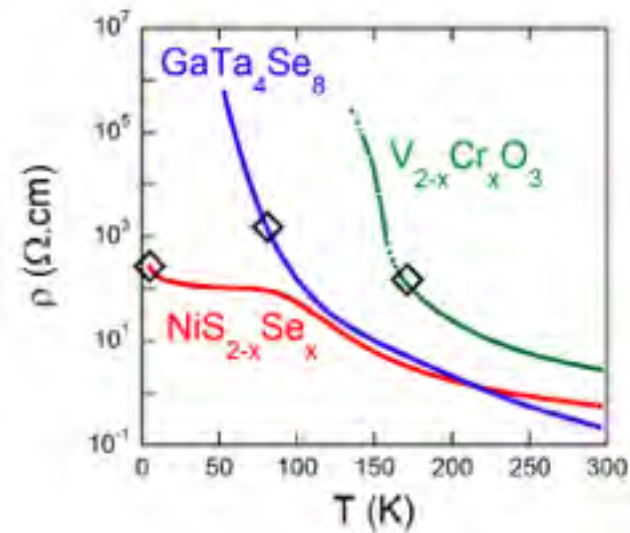
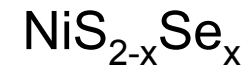
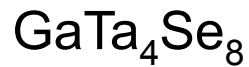
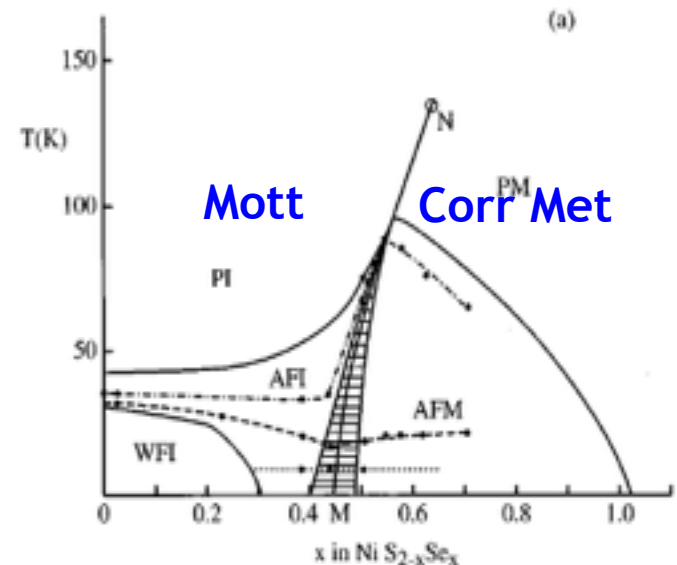
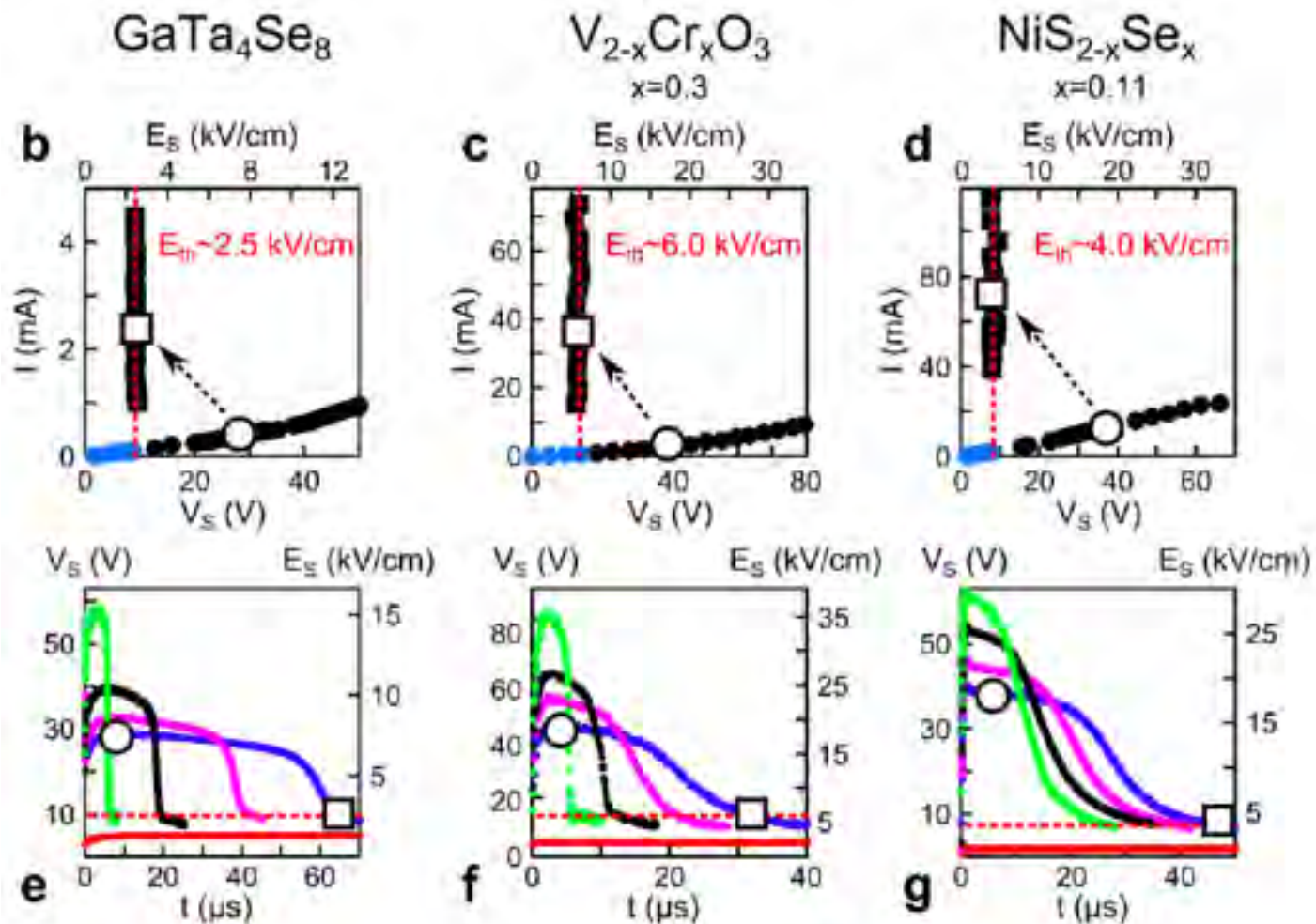


FIG. 70. Phase diagram for doped V_2O_5 ($\text{V}_{1-x}\text{Cr}_x$) $_2\text{O}_5$ and ($\text{V}_{1-x}\text{Ti}_x$) $_2\text{O}_5$. From McWhan *et al.*, 1973.



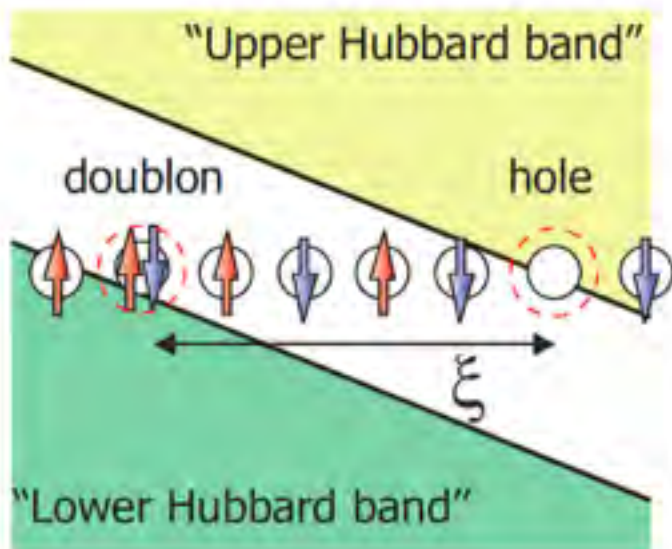
Czjzek *et al* JMMM '76

Universal behavior: three different Mott Insulators



What is the origin of the Mott electric-breakdown?

Hubbard model 1D

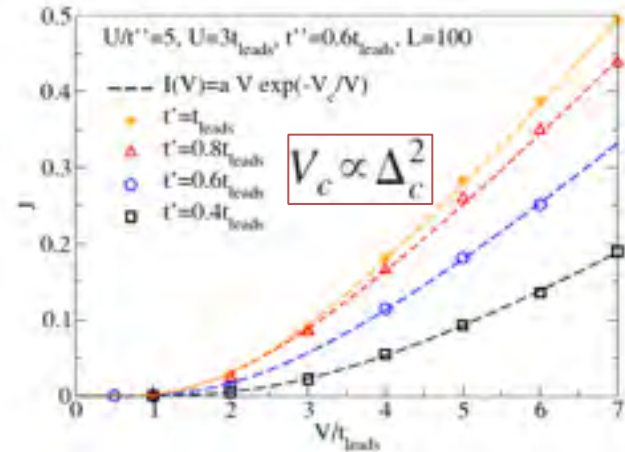


$$F_{\text{th}} \propto \Delta_{\text{Mott}}^2$$

$$1/\xi \sim \Delta_{\text{Mott}} \quad (1\text{D})$$

$$F_{\text{th}} \simeq \frac{\Delta_{\text{Mott}}}{2\xi}$$

$$J \sim \Gamma_p = \frac{F_0}{2\pi} \exp\left(-\pi \frac{F_{\text{th}}}{F_0}\right)$$



T. Oka et al. '03 '05 '10 '12
F. Heidrich-Meisner et al '10

M. Eckstein et al. '10 '11 (DMFT)
A. Amaricci et al. '12 (DMFT)

$$??? 1/\xi \sim \Delta_{\text{Mott}} \quad (3\text{D})$$

$$??? \xi \sim \mu\text{m} \quad (3\text{D})$$

$$\Delta \sim 10^{-1} \text{ eV}$$

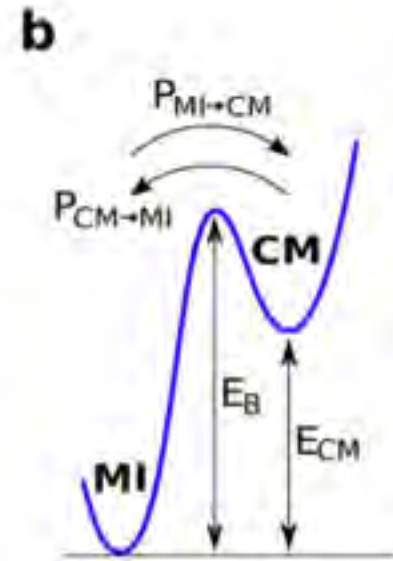
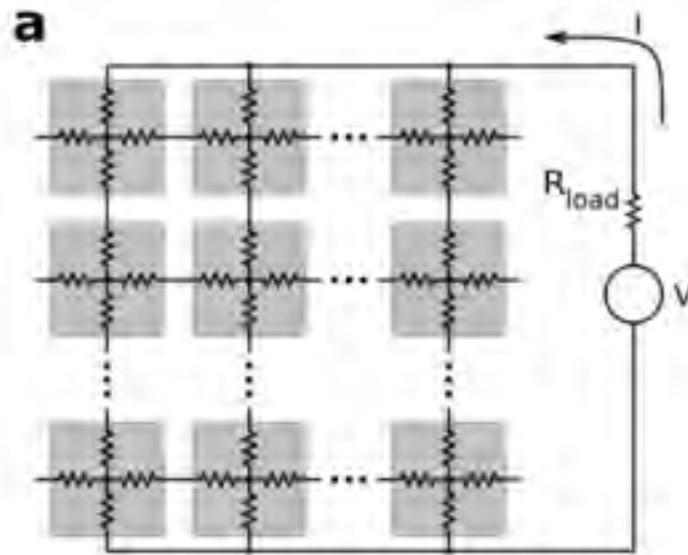
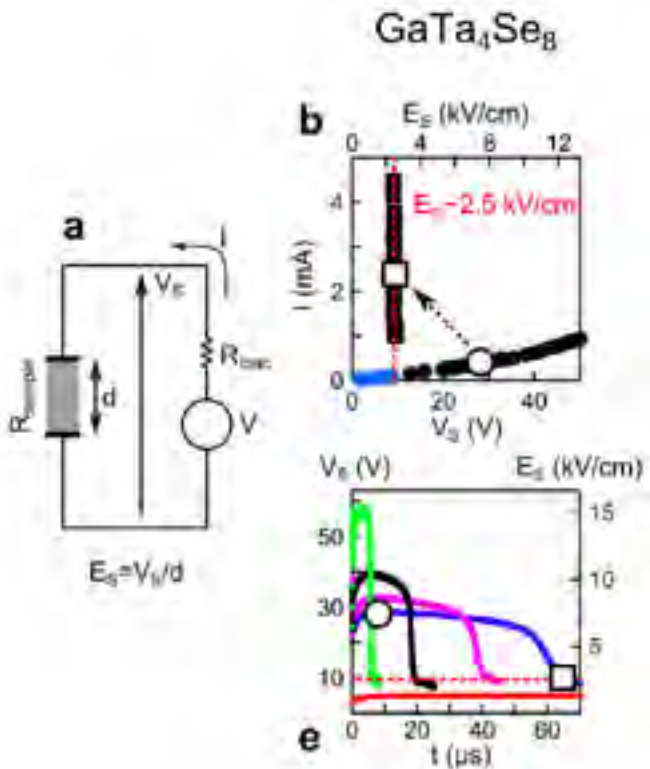
$$\xi \sim 1 \text{ nm} = 10^{-7} \text{ cm}$$

$$F_{\text{Th}} \sim 1 \text{ MV/cm}$$

$$E_{\text{Th}} \sim 1 \text{ KV/cm} \quad \text{!!!!}$$

Model of the Mott resistive transition

P. Stolar et al Adv. Mater. (2013)



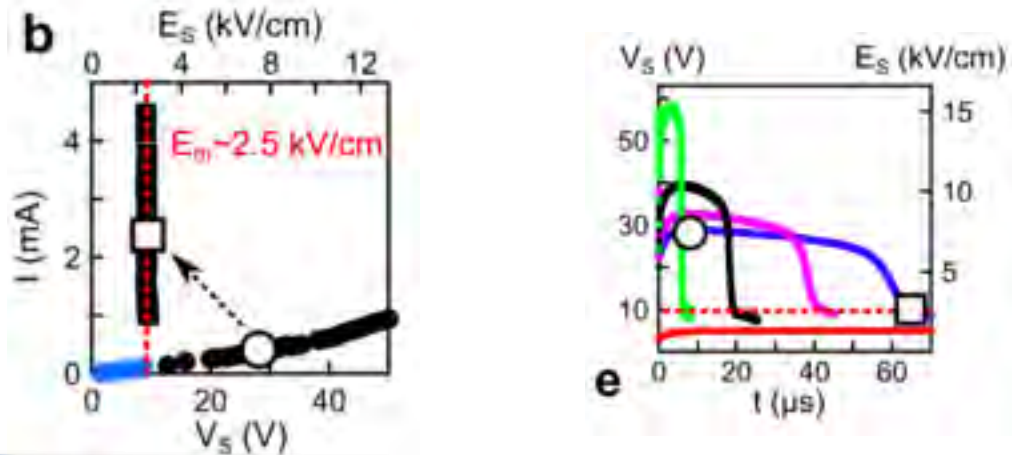
Two states: MI - Mott insulator
 CM - Correlated metal
 $R_{MI} \gg R_{CM}$

$P_{MI \rightarrow CM}$ and $P_{CM \rightarrow MI}$ are transition probabilities

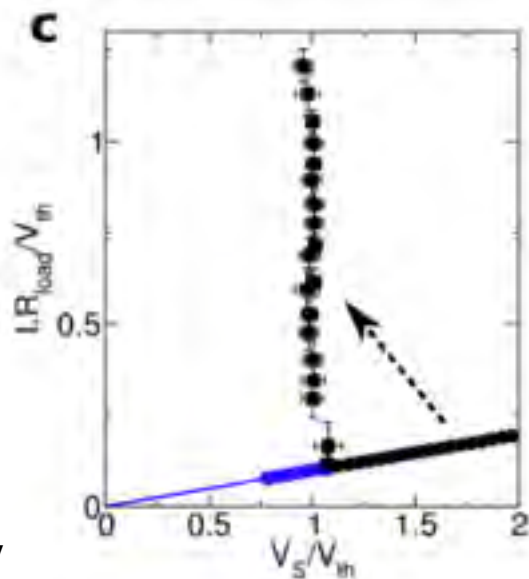
$$P_{MI \rightarrow CM} = v e^{-(E_B - q\Delta V)/kT} \quad P_{CM \rightarrow MI} = v e^{-(E_B - E_{CM})/kT}$$

Model results: Threshold Mott resistive transition

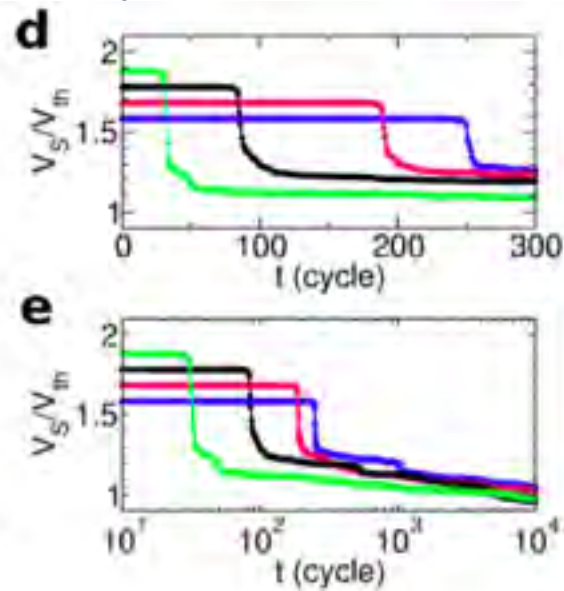
Experiment



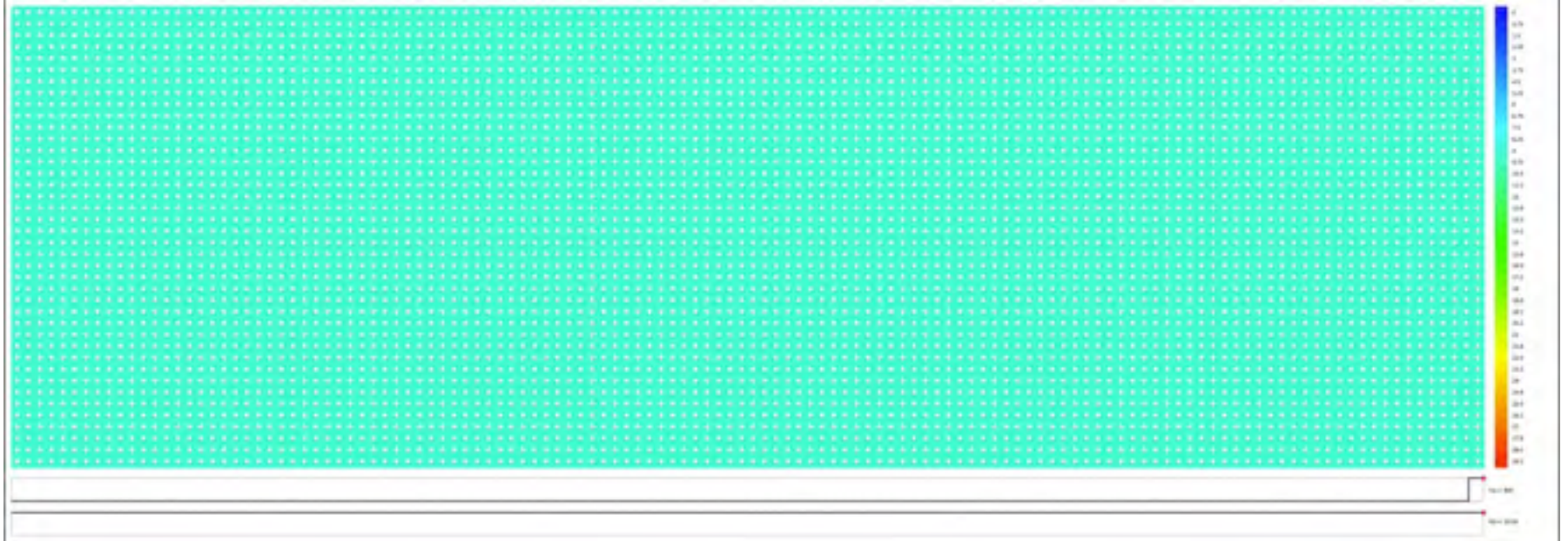
Theory



$$V_S/V_{Th} = 1.74, 1.84, 1.95, 2.06$$



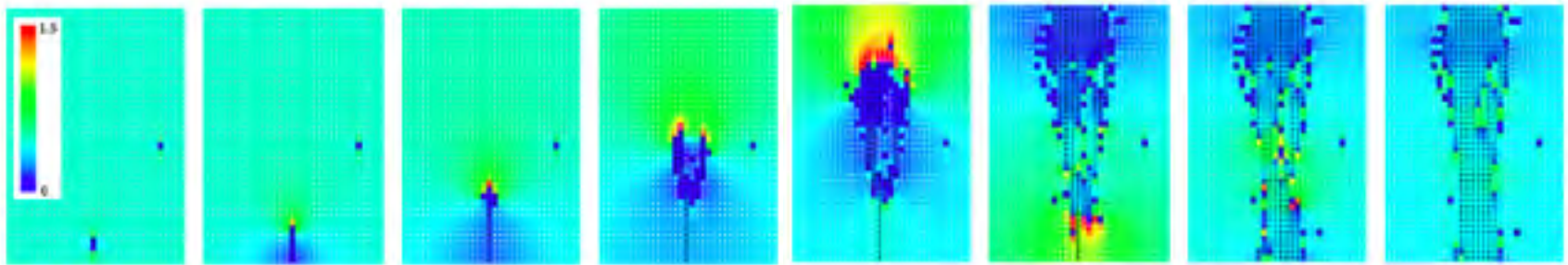
How the transition evolves in time?



Each pixel is a cell of the resistor network model

Color intensity indicates the local ΔV drops (ie local E)

How the transition evolves in time? (snapshots)



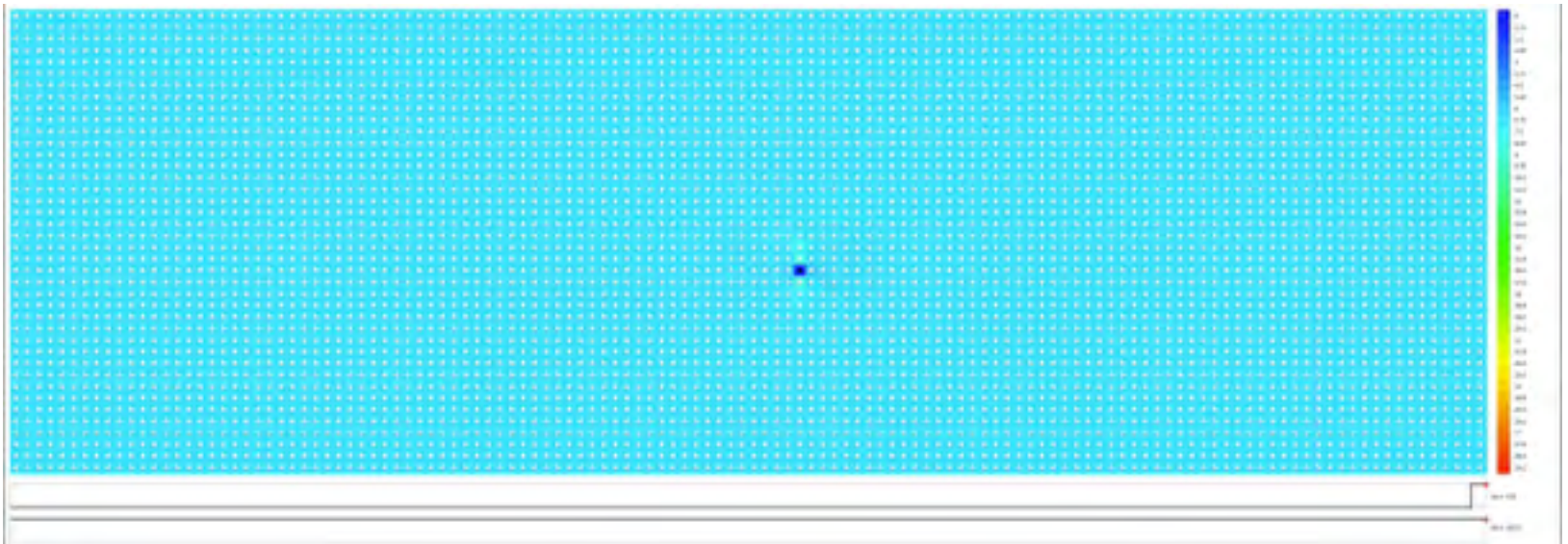
time \longrightarrow

Threshold effect

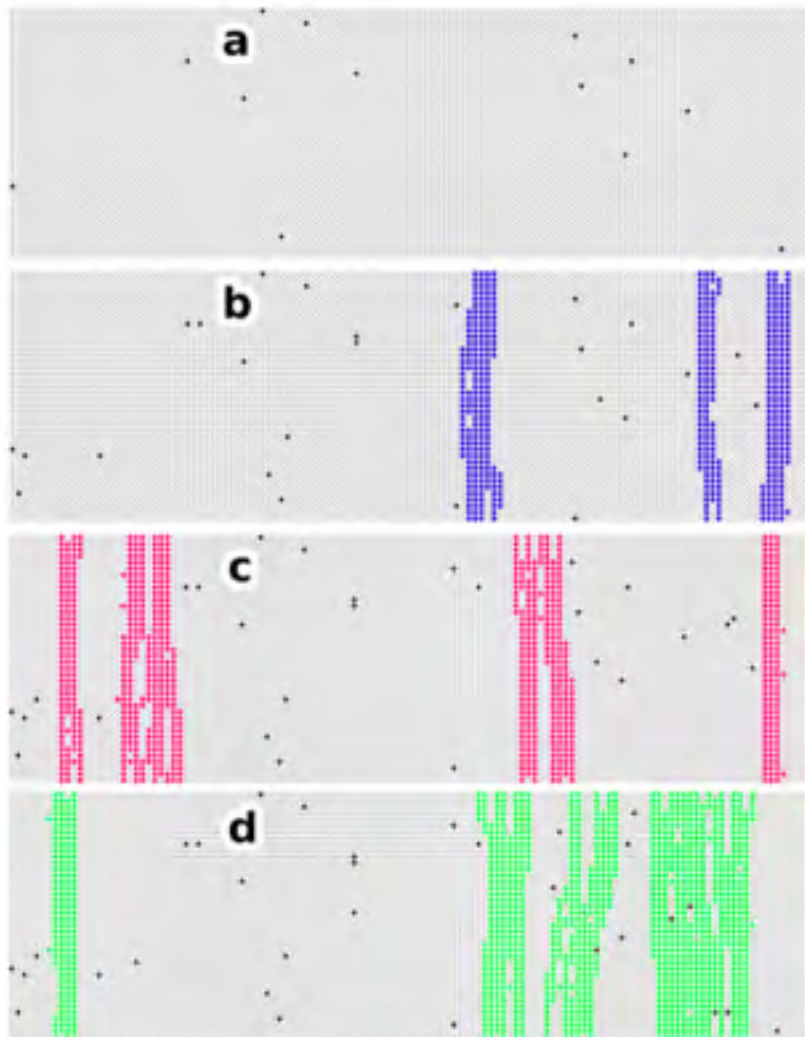
Below threshold



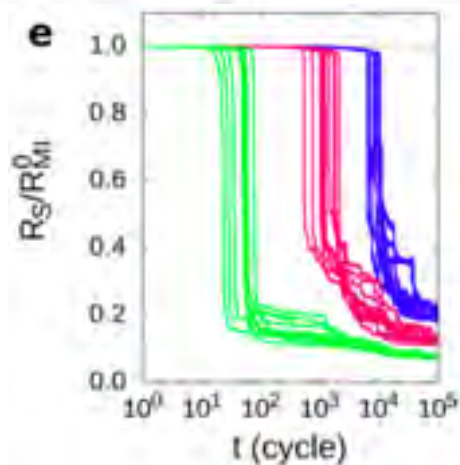
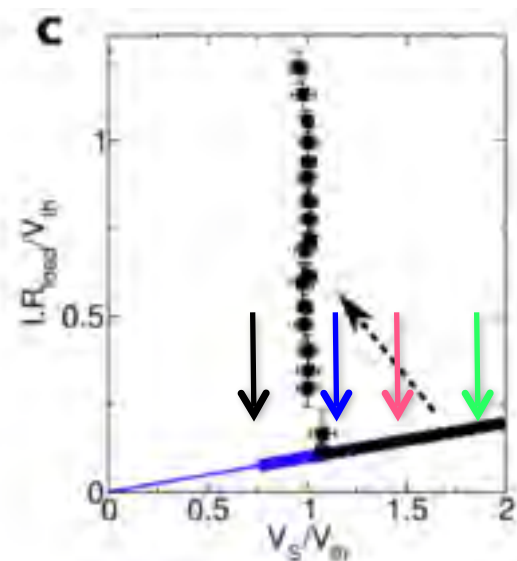
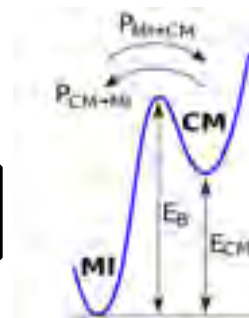
Above threshold



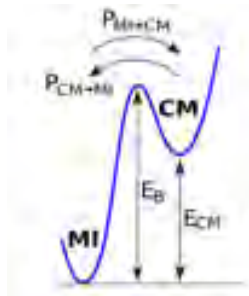
Threshold effect



$$V_S/V_{Th} = 0.7, 1.1, 1.4, 1.8$$



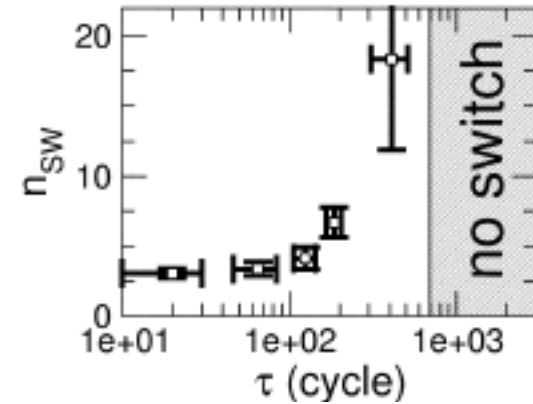
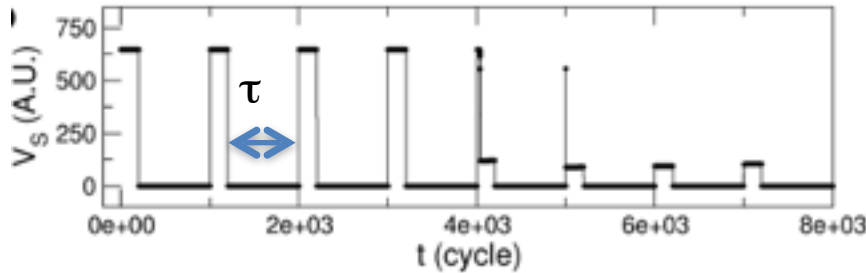
Model prediction: Neuromorphic behaviour!



Transition rates imply the existence of a relaxation time scale t_{relax}

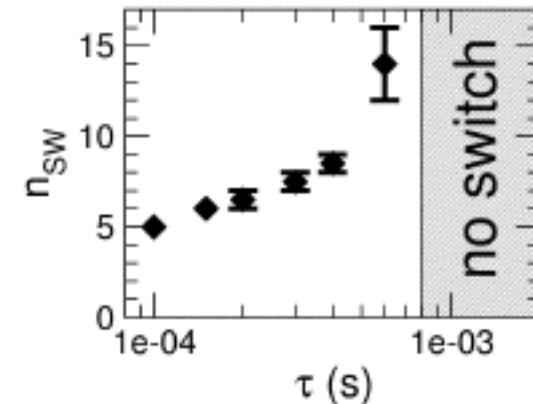
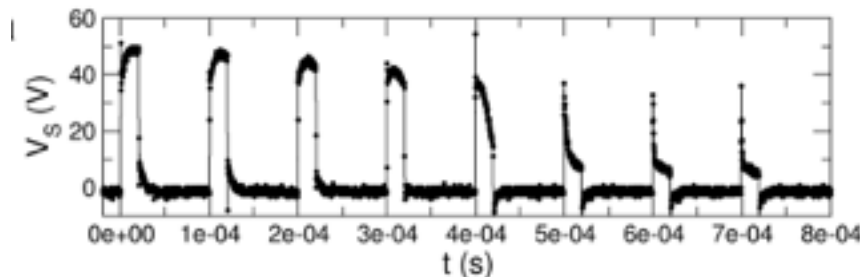
Short pulses ($< t_{delay}$) are sent at intervals $\tau < t_{relax}$

Model prediction



Transition after 5 pulses

Experiment



Summary

- GaTa_4Se_8 is a new Mott-Hubbard system
- E-field driven Mott insulators show a universal resistive transition with threshold behavior
- A phenomenological model based on DMFT Mott-Hubbard physics captures the qualitative behavior of the Mott resistive transition
- New electronic emergent behavior: neuromorphic

Refs:

V. Guiot et al, Nat Comm (2013)

P. Stoliar et al., Adv. Mat. (2013)

A. Camjayi et al., Phys Rev Lett (2014)

L. Cario et al Adv Func Mat (in press) **Review**