Aspen Center for Physics
Quantum Matter: Computation Meets Experiments

Hubbard model: Mott Transition and Quantum Critical

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University of Michigan

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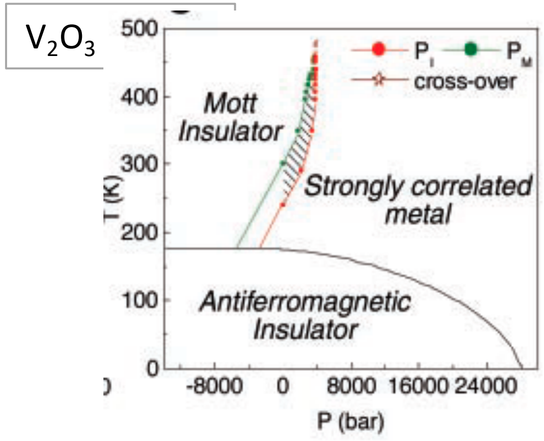
Oak Ridge Nat. Lab

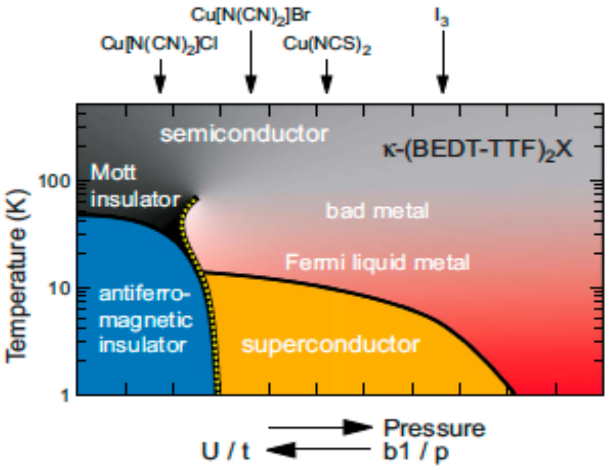
1. DMFT reveals Quantum Critical Scaling in Hubbard model

MIT a fundamental phenomenon occurring in various quantum systems

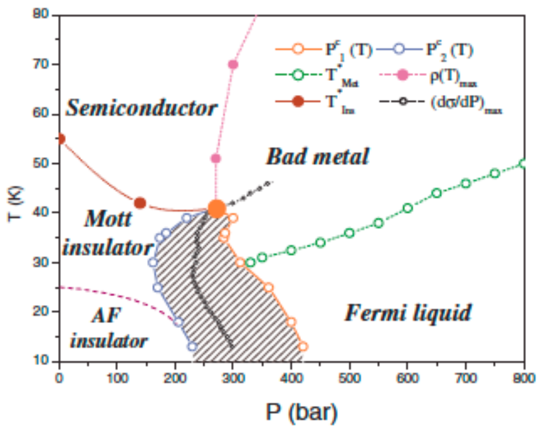
The Mott Metal-insulator transition is the central phenomena for many strongly correlated electron systems.



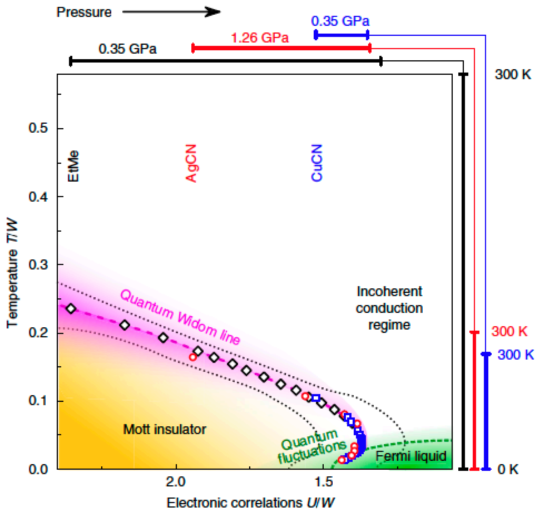
P. Limelette, et. al, Science 302, 3 (2003)



K. Kanoda et alNature, 436,2005



P. Limelette, et. al, PRL 91, 2003)



A. Pustogow, …, M. Dressell, Nature materials, 17, 2018.

-Interaction driven first order Mott Metal-insulator transition;

-Tc is often smaller than other energy scales, Tc <<U <<W<< Ef

A many-body quantum systems on the verge of instability between two competing ground states may exhibit QC phenomena.

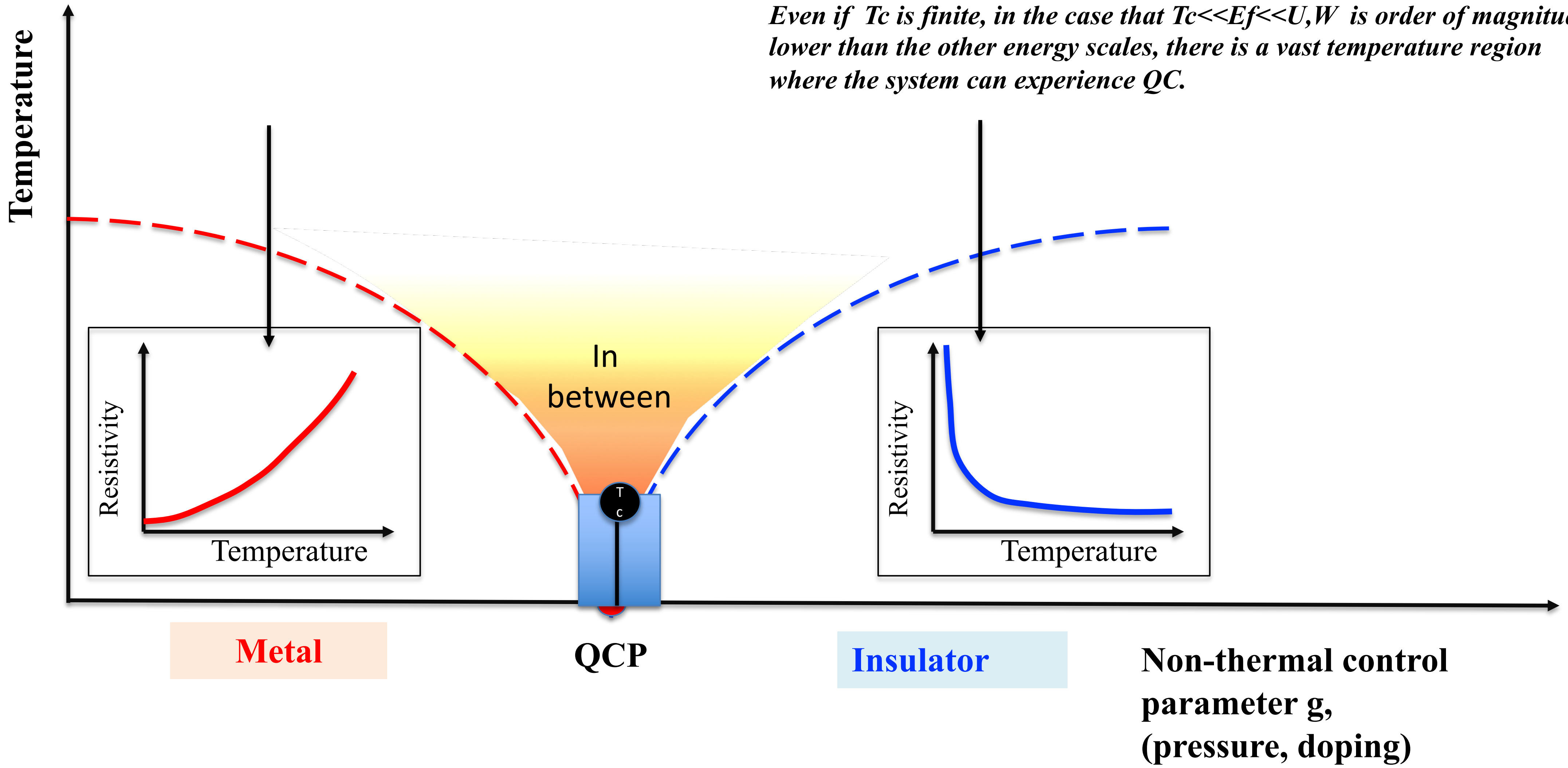
$$H=-\sum_{\langle ij\rangle,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}$$

Question: what are the universal featured of correlated MIT? Is there a possibility of Quantum Phase Transition in Mott Insulators.

MIT a Quantum Critical Prospective

A many-body quantum systems on the verge of instability between two competing ground states may exhibit QC phenomena.

Even if Tc is finite, in the case that Tc<<Ef<<U,W is order of magnitude lower than the other energy scales, there is a vast temperature region where the system can experience QC.

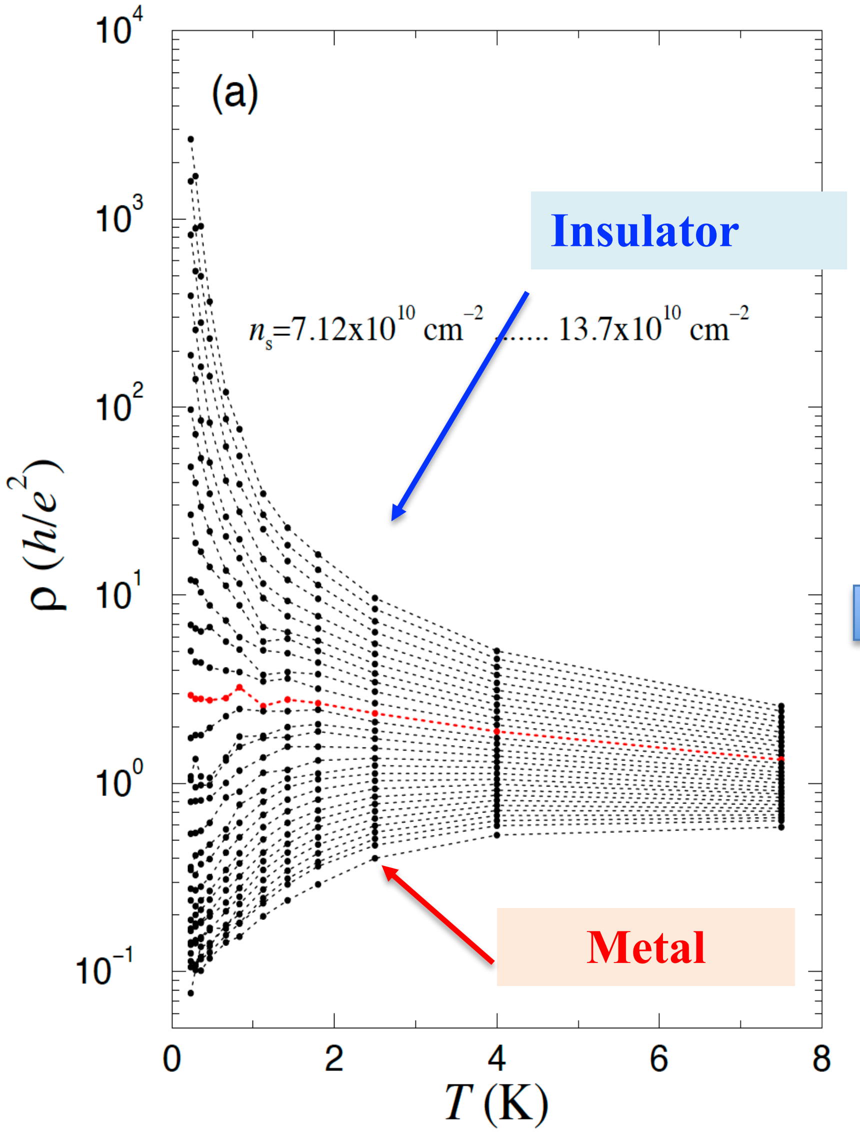


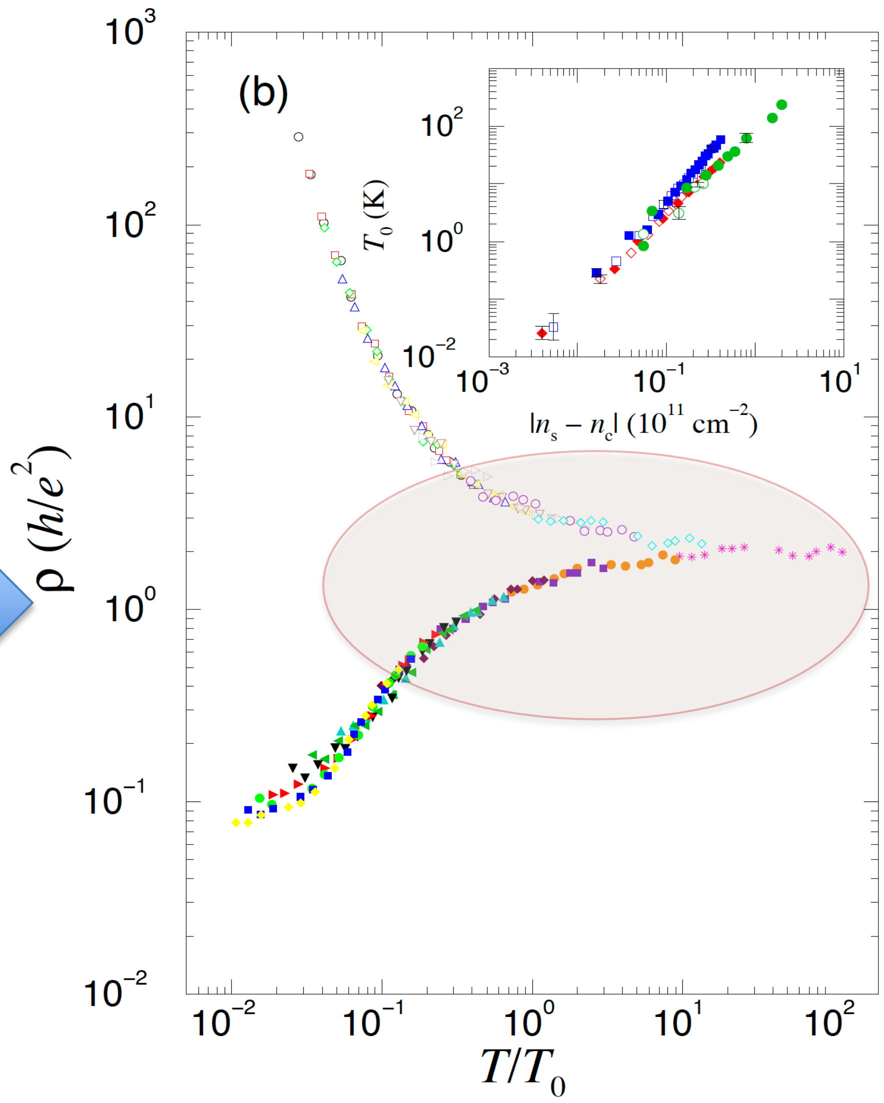
Quantum Critical Scaling in 2D MOSFETs MIT
Kravchenko, Sarachik; D. Ppopovic 1995, 1997

PHYSICAL REVIEW B VOLUME 51, NUMBER 11 15 MARCH 1995-I

Scaling of an anomalous metal-insulator transition in a two-dimensional system in silicon at $B=0$

S. V. Kravchenko, Whitney E. Mason, G. E. Bowker,* and J. E. Furneaux
Laboratory for Electronic Properties of Materials and Department of Physics and Astronomy, University of Oklahoma, Norman, Oklahoma 73019





$$\rho(n_s, T) = \rho_c(T)F(T/\delta n^{z\nu})$$

- Resistivity curves can be collapsed into two branches;
- Scaling parameter T_0 vanishes on both sides on MIT with the same exponents;
- Scaled curves exhibit mirror symmetry

$$\rho(\delta n_s, T) = 1/\rho(-\delta n_s, T)$$

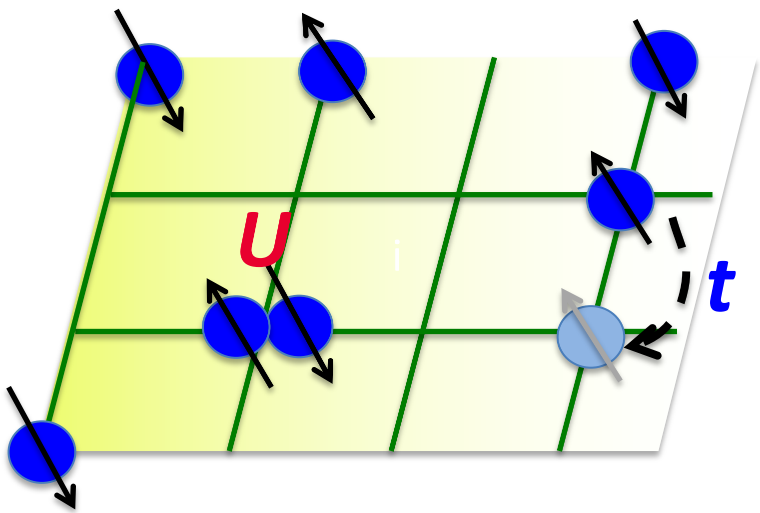
V. Dobrosavljevic et al, prl 1997: mirror symmetry of scaled curves→ transition is a strong coupling phenomena: how insulator is being destroyed.

Theory prospective

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

kinetic term describes electron hopping

potential energy term describes (screened) Coulomb repulsion



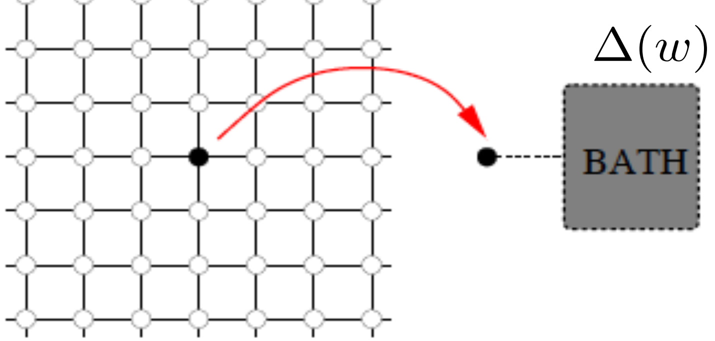
Main components: competition between itinerancy of electron favored by KE (t-hopping term) and **the localization of electrons** due to Coulomb interaction U.

A. Georges et al., Rev. Mod. Phys. 68, 13 (1996)

Local

$$
\boxed{\Sigma(k,w) \approx \Sigma(w)}
$$

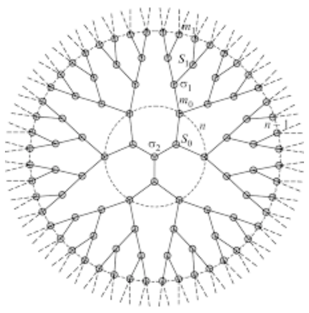
DMFT



DMFT; Georges et al., Rev. Mod. Phys. 68, 13 (1996)

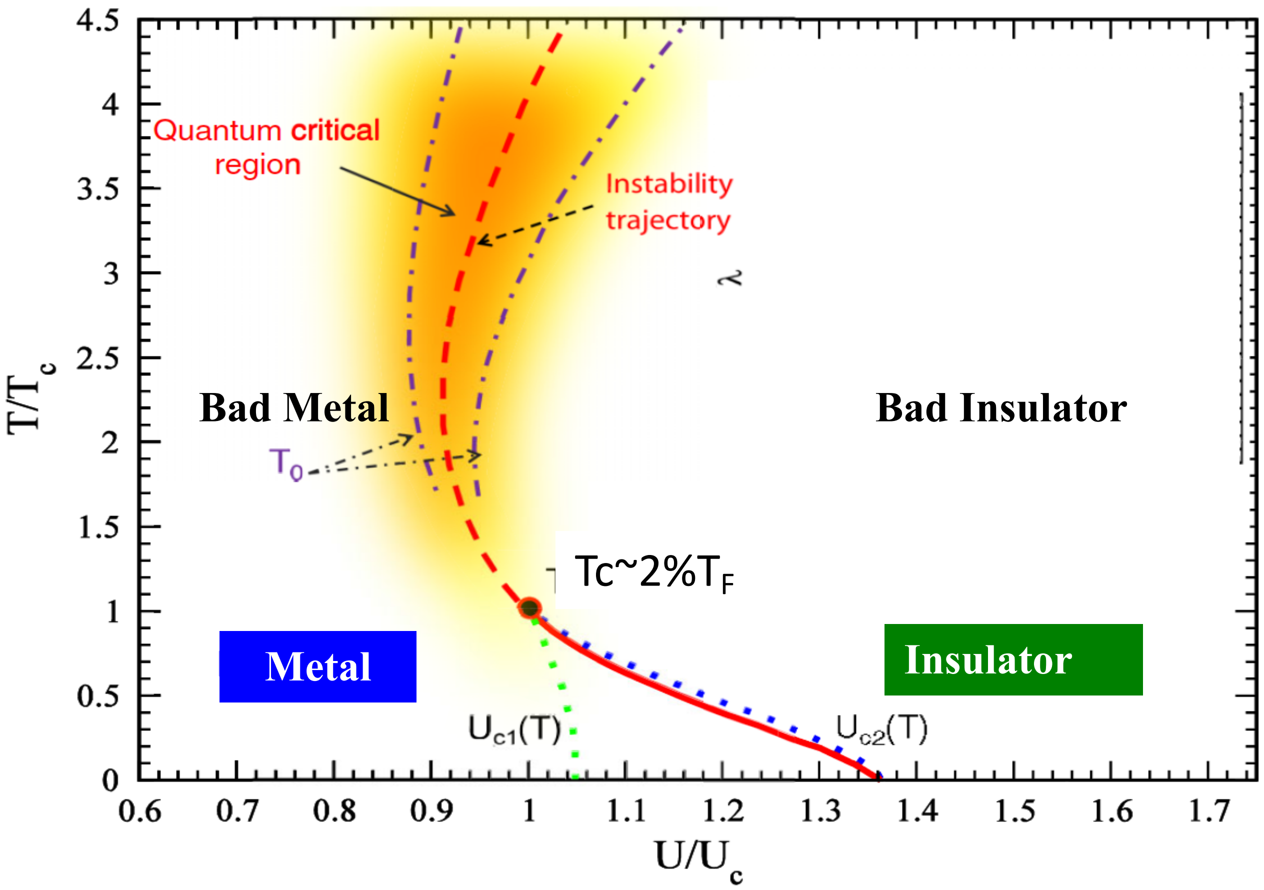
T. Maier, Quantum cluster theorties, RMP, 2005.

Park, Haule, Kotliar, PRL 101, 186403 (2008).



Quantum Critical Behavior in High Temperature regime

H.T. et.al, Phys. Rev. Lett. 107, 026401 (2011), Phys. Rev. B 88, 075143 (2013)



QC Regime revealed via scaling of High Temperature Transport.

Details on revealing Quantum Critical Behavior in High Temperature regime

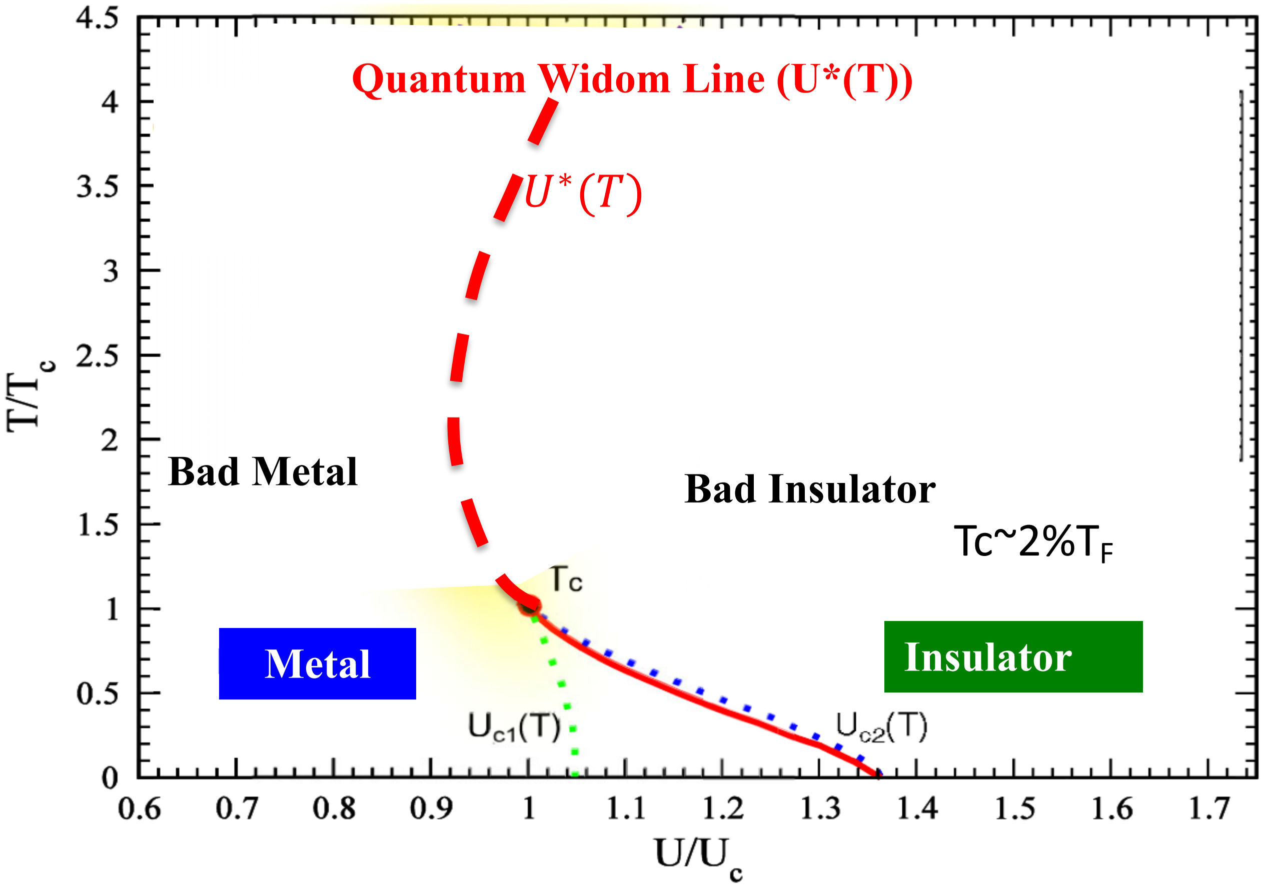
H.T. et.al, Phys. Rev. Lett. 107, 026401 (2011), Phys. Rev. B 88, 075143 (2013)

H.T.

V. Donbrosavljevic

High Temperature Regime

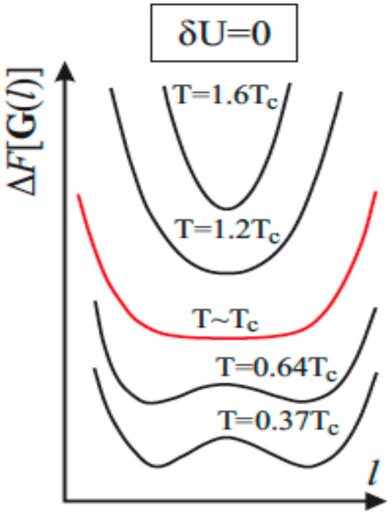
Also work by Sordi … Tremblay , Scientific Reports 2, 547, (2012); PRB 87, 041101(R) (2013),



Ben Widom

To reveal the proper scaling behavior→ follow a set of trajectories parallel to instability trajectory "Widom line".

Determined from the examining the curvature of the corresponding free energy functional:
0 at Tc, and finite and minimal at T>Tc.

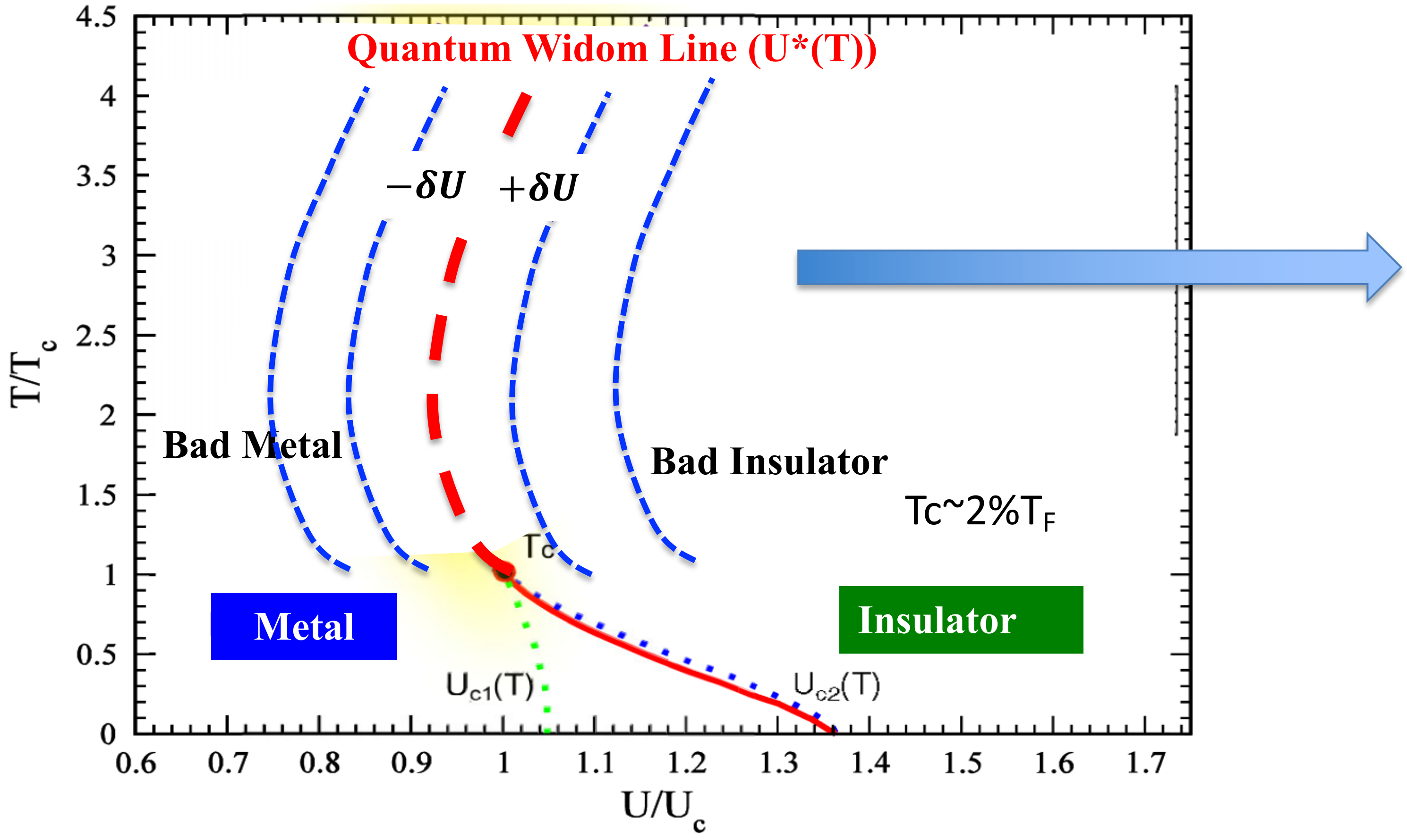


H.T.

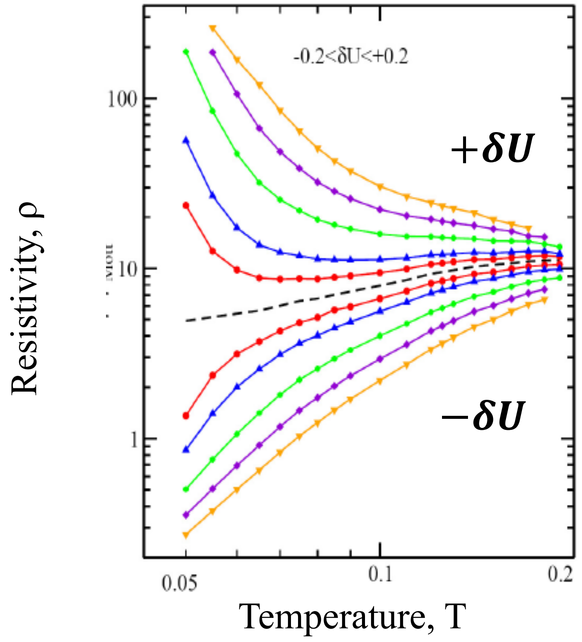
V. Donbrosavljevic

Quantum Critical Behavior in High Temperature regime

H.T. et.al, Phys. Rev. Lett. 107, 026401 (2011), Phys. Rev. B 88, 075143 (2013)



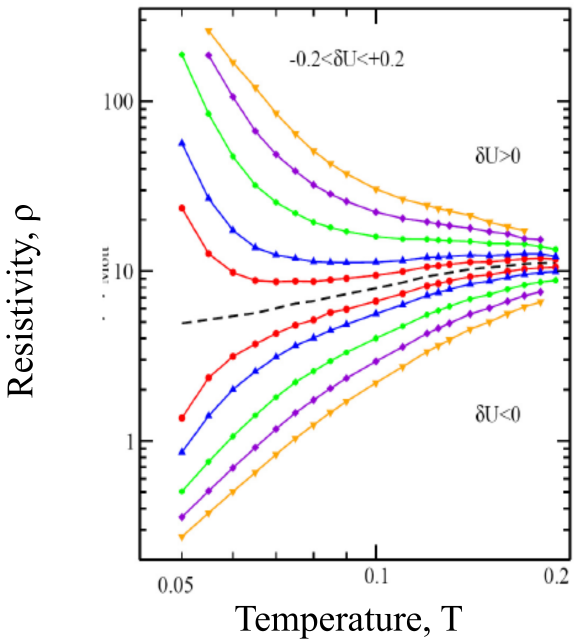
Transport along $\delta U = U - U^*$



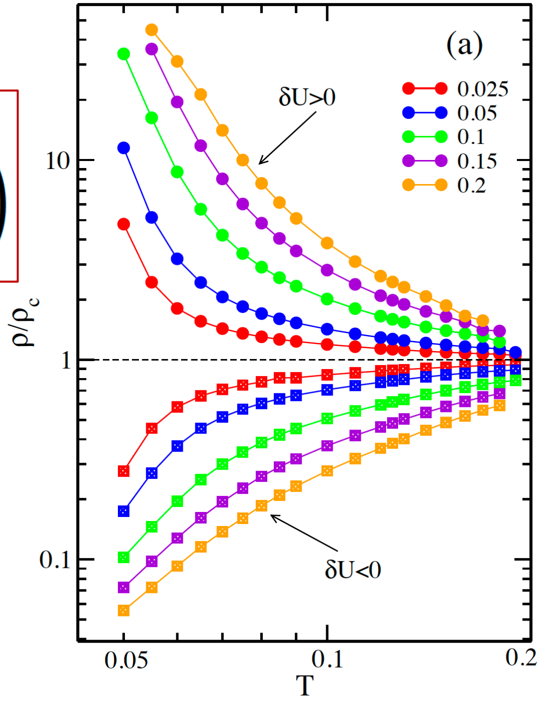
Signatures of Quantum Criticality: Quantum Scaling

H.T. et.al, PRL 107, 026401 (2011; PRB 2013

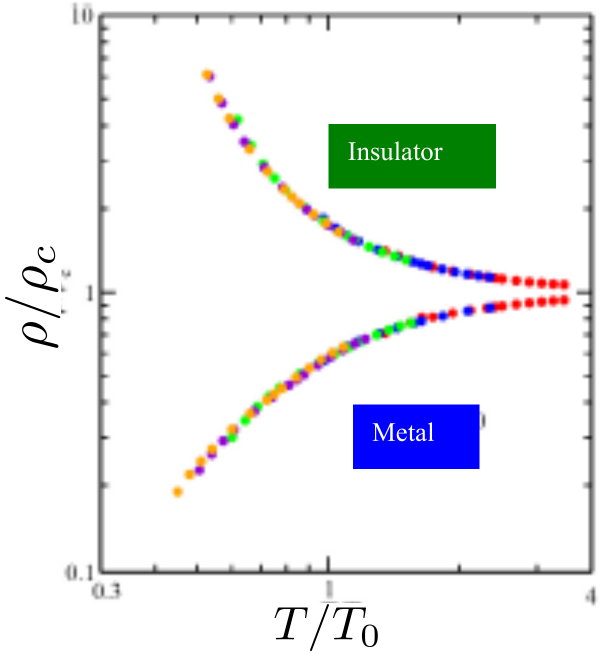
Raw data



$$\frac{\rho(\delta U,T)}{\rho_c(T)} = f_{\pm}\left(\frac{T}{|\delta U|^{\nu z}}\right)$$

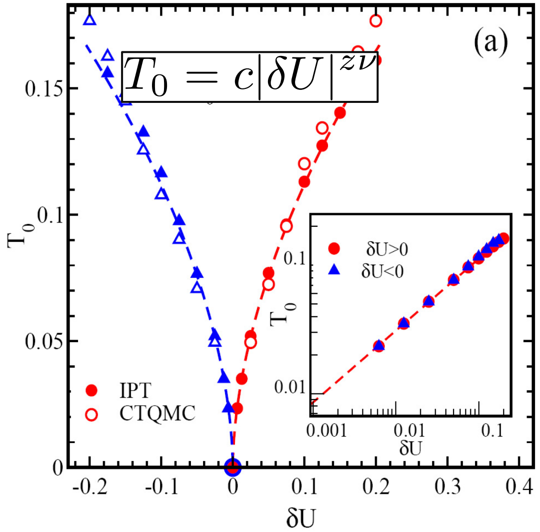


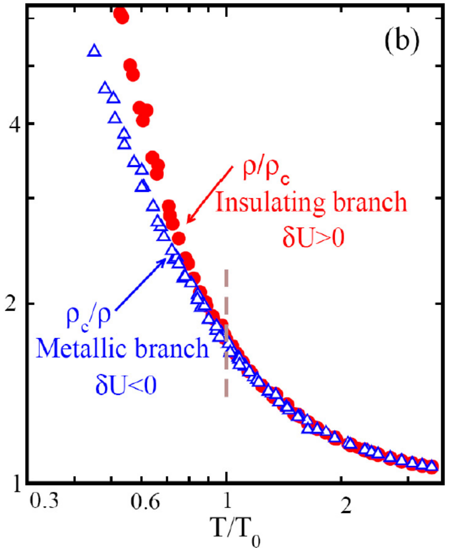
Scaled data

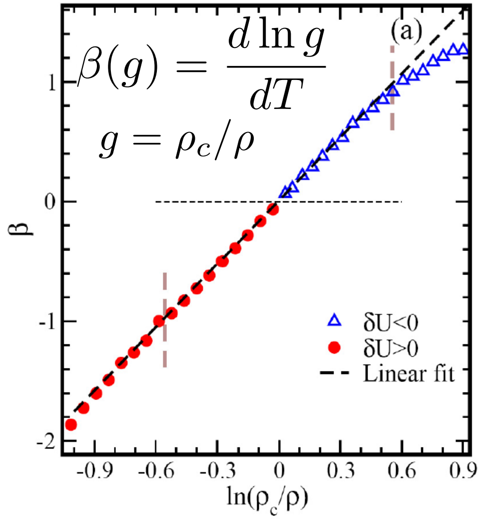


Features of Quantum Criticality

- **Power law behavior of scaling parameter;**
- **The same scaling exponents for M and I branches: zν~0.57.**
- **Mirror symmetry** of scaled curves.
- Scaling function is **continuous** through the transition; ~lng→ **strong coupling nature of the critical point**, governed by the same processes as insulating behavior.





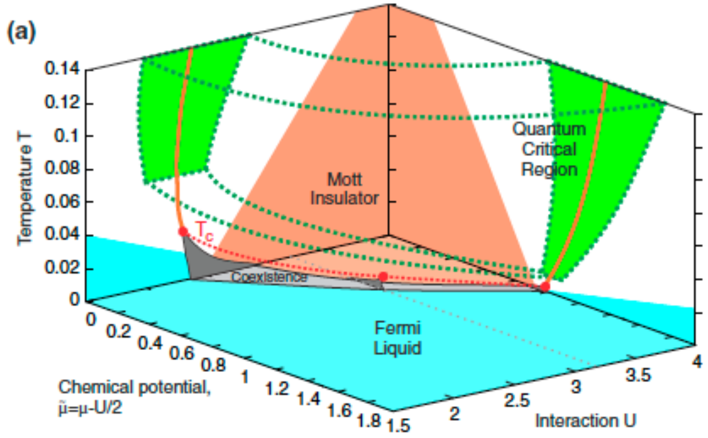


QC Scaling in doped Hubbard model

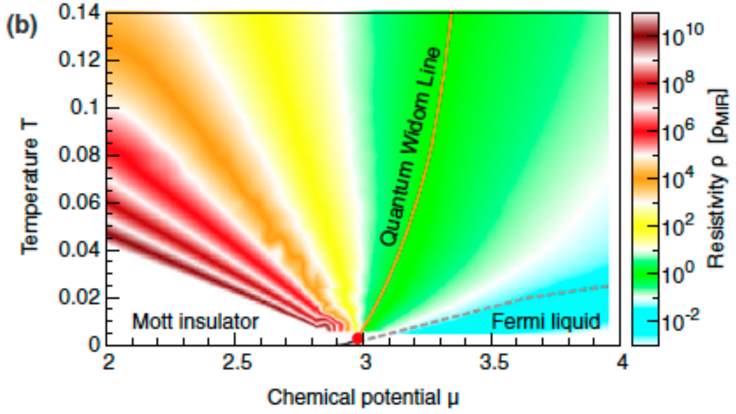
PRL **114**, 246402 (2015) PHYSICAL REVIEW LETTERS week ending 19 JUNE 2015

Bad-Metal Behavior Reveals Mott Quantum Criticality in Doped Hubbard Models

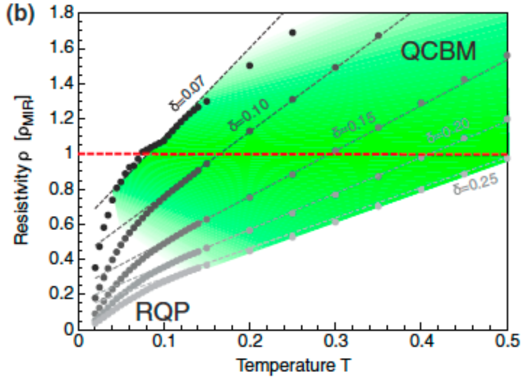
J. Vučičević,[1] D. Tanasković,[1] M. J. Rozenberg,[2] and V. Dobrosavljević[3]



Tc and coexistence region get suppressed under doping.



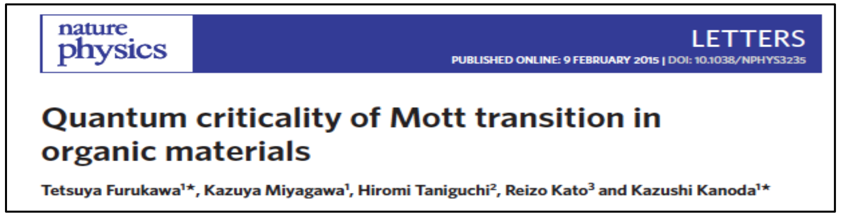
QC scaling persists even to a wider parameter regime. zv=1.35.



QC region is covering the entire bad metal regime.

Computation meets Experiments

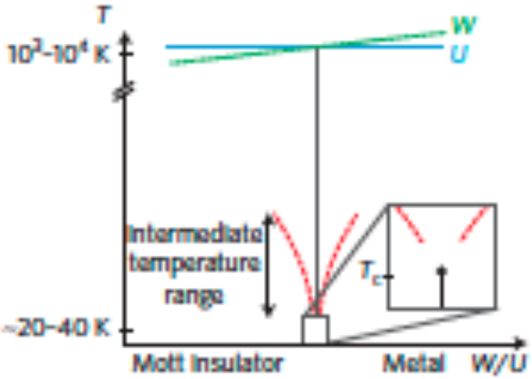
2. DMFT-predicted quantum critical scaling of transport has been confirmed experimentally!

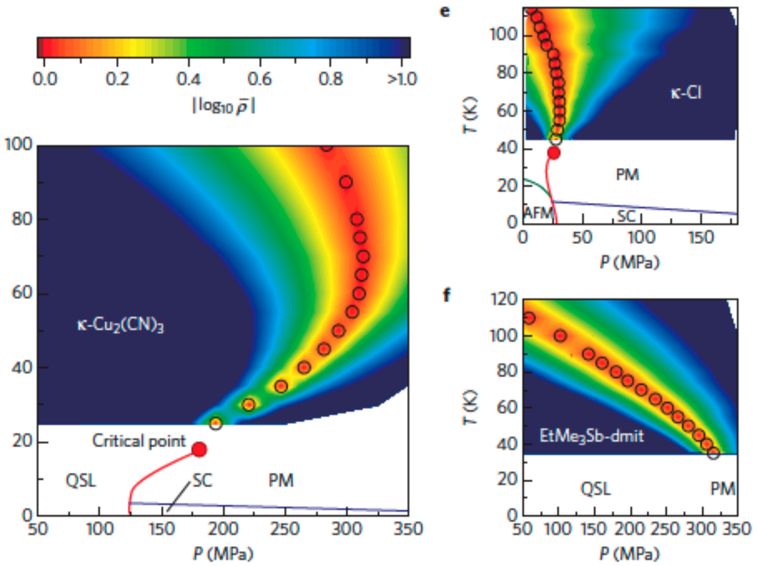

nature physics | LETTERS

PUBLISHED ONLINE: 9 FEBRUARY 2015 | DOI: 10.1038/NPHYS3235

Quantum criticality of Mott transition in organic materials

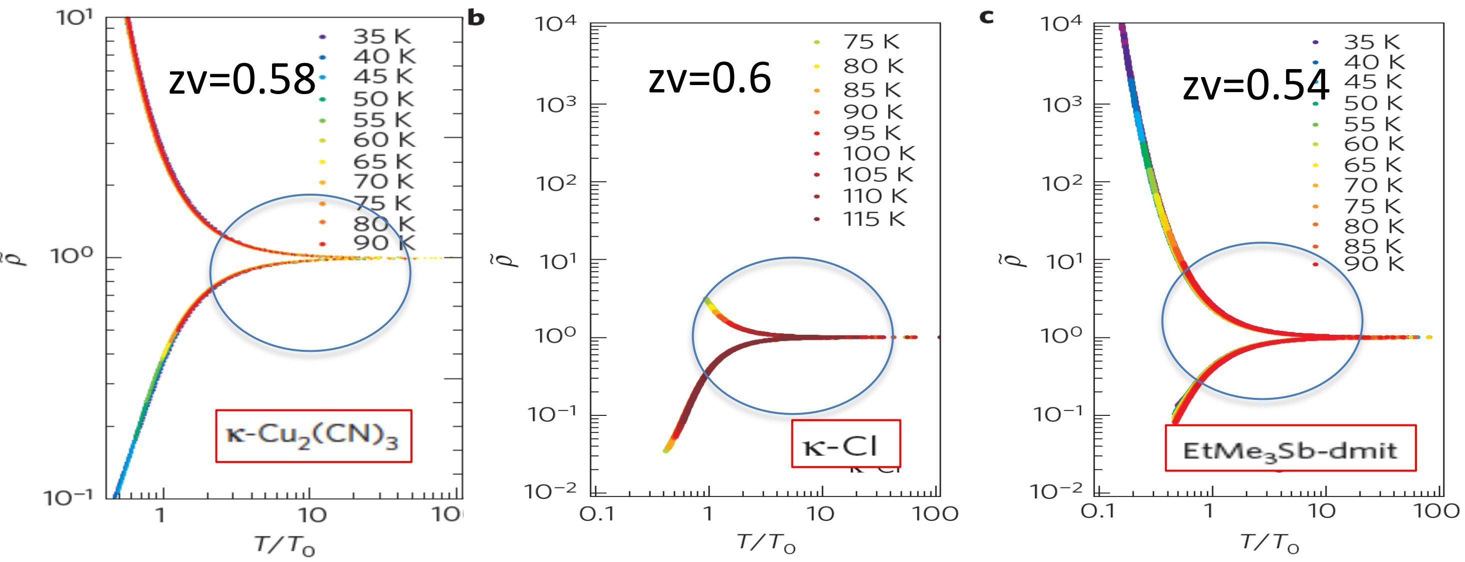
Tetsuya Furukawa[1]*, Kazuya Miyagawa[1], Hiromi Taniguchi[2], Reizo Kato[3] and Kazushi Kanoda[1]*





Experiment

T. Furukawa …. K. Kanoda, Nature Physics, 11 211, (2015).



The experimental scaling features coincides with those of DMFT.

1) DMFT=0.57; Exp. Critical: 0.58, 0.6, 0.54.
2) Bow-banded shape of Widom line;
3) Fan-shaped QC scaling region 2Tc<T<4Tc;
4) Power law of scaling parameter; Mirror symmetry;

Material independent universal quantum critical behavior in high temperature regime.

Different types of Mott transition in three systems: QSL-SC, AFM-SC, QSL-PM.

QC in disordered systems

Experiment

PHYSICAL REVIEW B **99**, 245139 (2019)

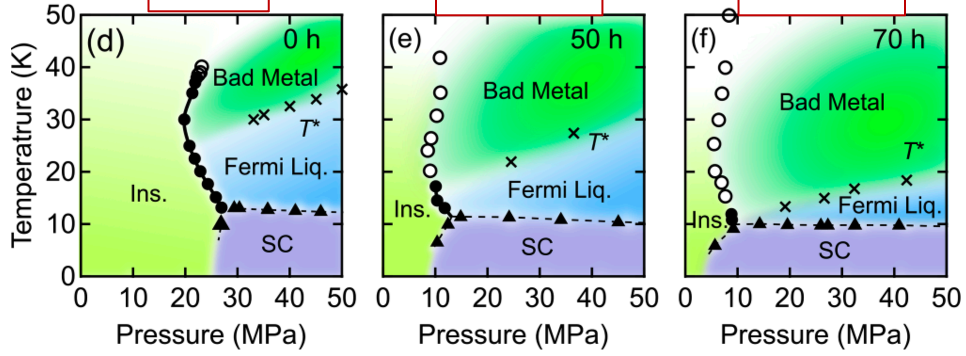
Disorder unveils Mott quantum criticality behind a first-order transition in the quasi-two-dimensional organic conductor κ-(ET)$_2$Cu[N(CN)$_2$]Cl

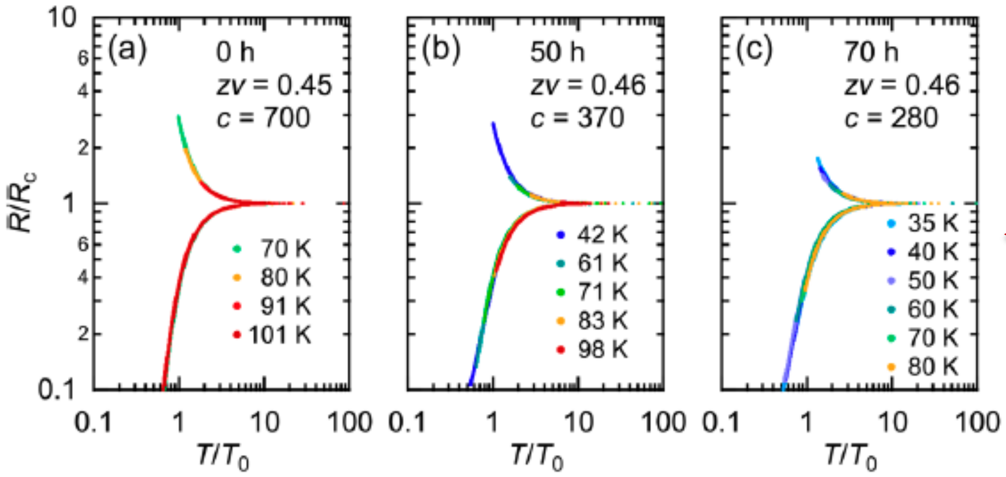
Mizuki Urai,[1] Tetsuya Furukawa,[2] Yasuhide Seki,[1] Kazuya Miyagawa,[1] Takahiko Sasaki,[3] Hiromi Taniguchi,[4] and Kazushi Kanoda[1]

clean

disorder

disorder



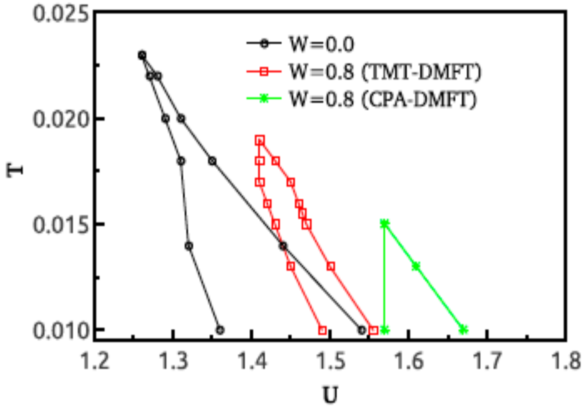


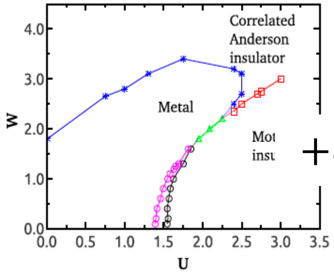
Theory

PHYSICAL REVIEW B **92**, 125143 (2015)

Anderson localization effects near the Mott metal-insulator transition

Helena Bragança,[1] M. C. O. Aguiar,[1] J. Vučičević,[2] D. Tanasković,[2] and V. Dobrosavljević[3]





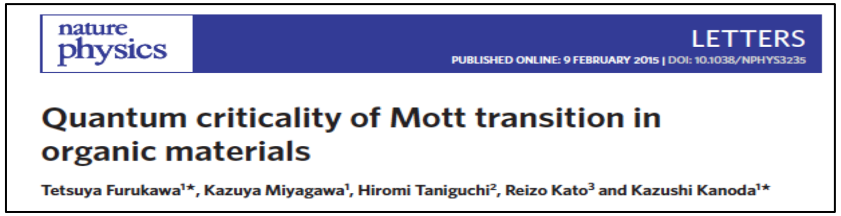
$+\delta U$

Tc gets suppressed by disorder
Uc for MIT is pushed to larger U

- -Tc gets suppressed by disorder
- -Coexistence region shrinks
- -FL is suppressed
- -QC scaling persists in disordered systems, exponents stay the same

Experimental Confirmation of QC scaling in four experiments

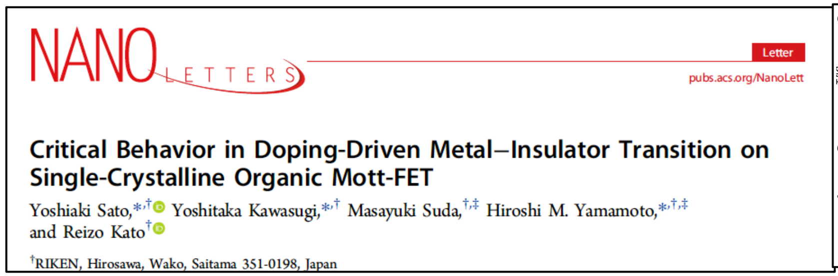
2015: QC scaling in three organic Mott material


nature physics
LETTERS
PUBLISHED ONLINE: 9 FEBRUARY 2015 | DOI: 10.1038/NPHYS3235

Quantum criticality of Mott transition in organic materials

Tetsuya Furukawa[1]*, Kazuya Miyagawa[1], Hiromi Taniguchi[2], Reizo Kato[3] and Kazushi Kanoda[1]*

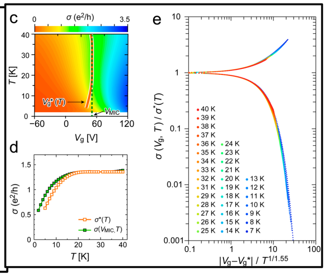
2017: QC Scaling in doped Mott Insulators


NANO LETTERS
Letter
pubs.acs.org/NanoLett

Critical Behavior in Doping-Driven Metal−Insulator Transition on Single-Crystalline Organic Mott-FET

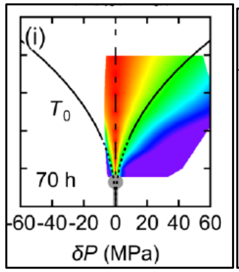
Yoshiaki Sato,*[†] Yoshitaka Kawasugi,*[†] Masayuki Suda,[†,‡] Hiroshi M. Yamamoto,*[†,‡] and Reizo Kato[†]

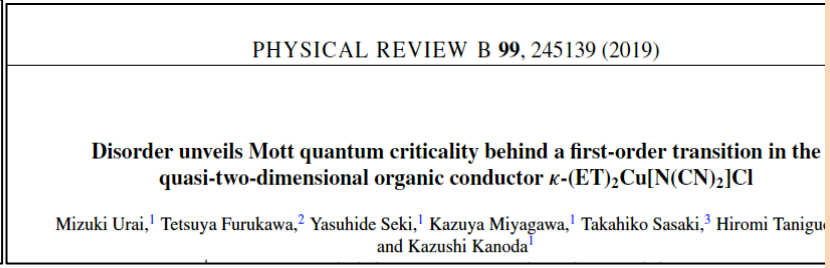
[†]RIKEN, Hirosawa, Wako, Saitama 351-0198, Japan



High temperature Mott Quantum Critical crossover a ubiquitous universal feature of various types of Mott transitions

2019: Disorder reveals QC in organic systems




PHYSICAL REVIEW B **99**, 245139 (2019)

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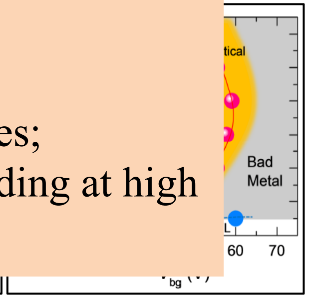
and Kazushi Kanoda[1]

2019-20: QC Scaling in transition-metal dichalcogenides.

Universal features of 2D MIT:

- 1rst order displaying phase coexistence;
- Tc<< Ef, the behavior in T>>Tc features QCS of resistivity curves;
- The QCR is centered around QWL with characteristic back-bending at high Tc.

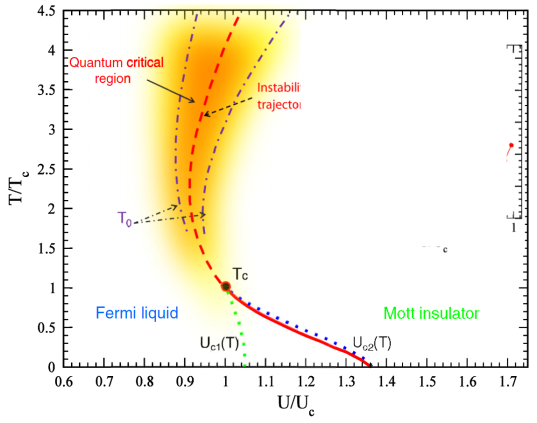


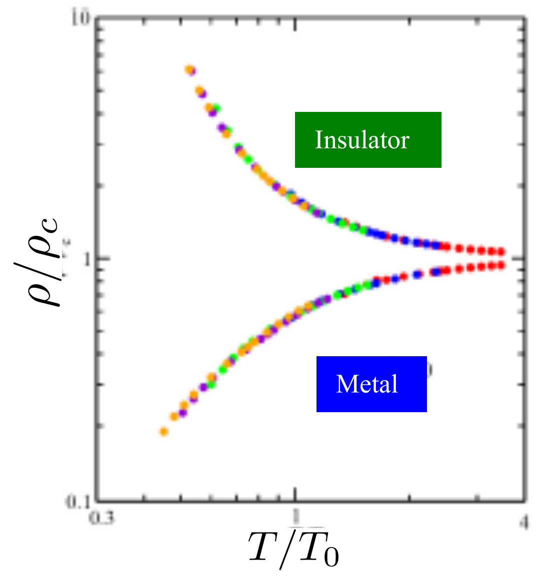
PRL 107, 026401 (2011) PHYSICAL REVIEW LETTERS week ending 8 JULY 2011

Quantum Critical Transport near the Mott Transition

H. Terletska,[1] J. Vučičević,[2] D. Tanasković,[2] and V. Dobrosavljević[1]

QC via Scaled of Transport



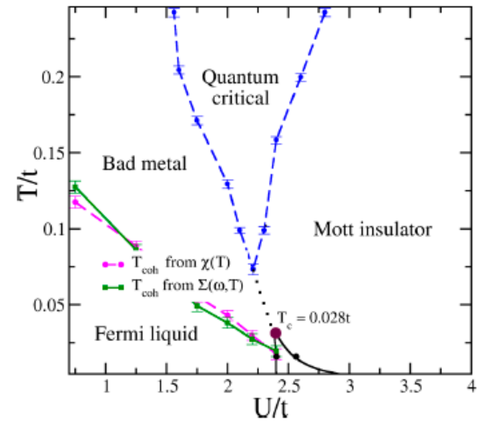


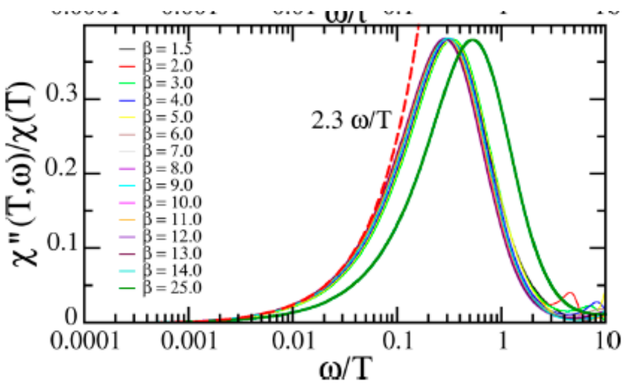
PHYSICAL REVIEW B 95, 165105 (2017)

Quantum critical local spin dynamics near the Mott metal-insulator transition in infinite dimensions

Nagamalleswararao Dasari,[1,*] N. S. Vidhyadhiraja,[1] Mark Jarrell,[2,3] and Ross H. McKenzie[4,†]

QC via Scaled of local Susceptibility





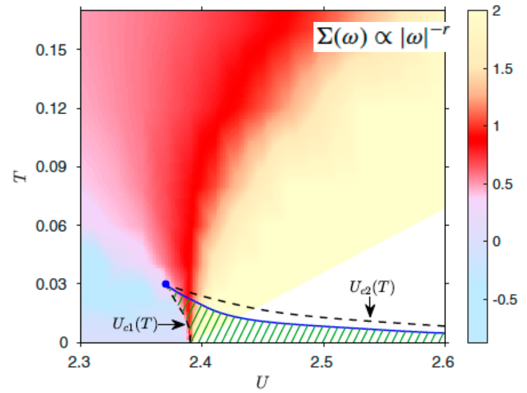
The local spin susceptibility was reported from DMFT to show ω/T scaling at fixed U in the regime above the critical endpoint.

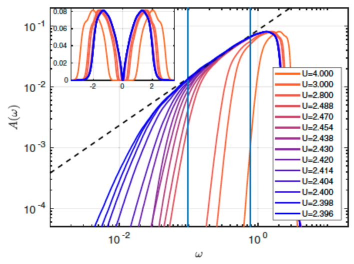
PHYSICAL REVIEW B 100, 155152 (2019)

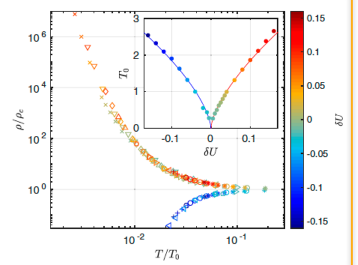
Mott quantum criticality in the one-band Hubbard model: Dynamical mean-field theory, power-law spectra, and scaling

Heike Eisenlohr,[1] Seung-Sup B. Lee,[2] and Matthias Vojta[1]

QC via power-law spectra and scaling







-A crossover power-law behavior in spectral function and self-energy is present at low and hig. temperatures.

-Resistivity scaling is found both above and below Tc.

-This **behavior is traced back to the metastable insulating behavior** in the coexistence region, suggesting local quantum criticality of Mott transition below Tc.

Some broader implications

- Excellent agreement of DMFT and experimental results at high temperature regimes suggest that dominant correlation physics in the regime above the Tc is local.

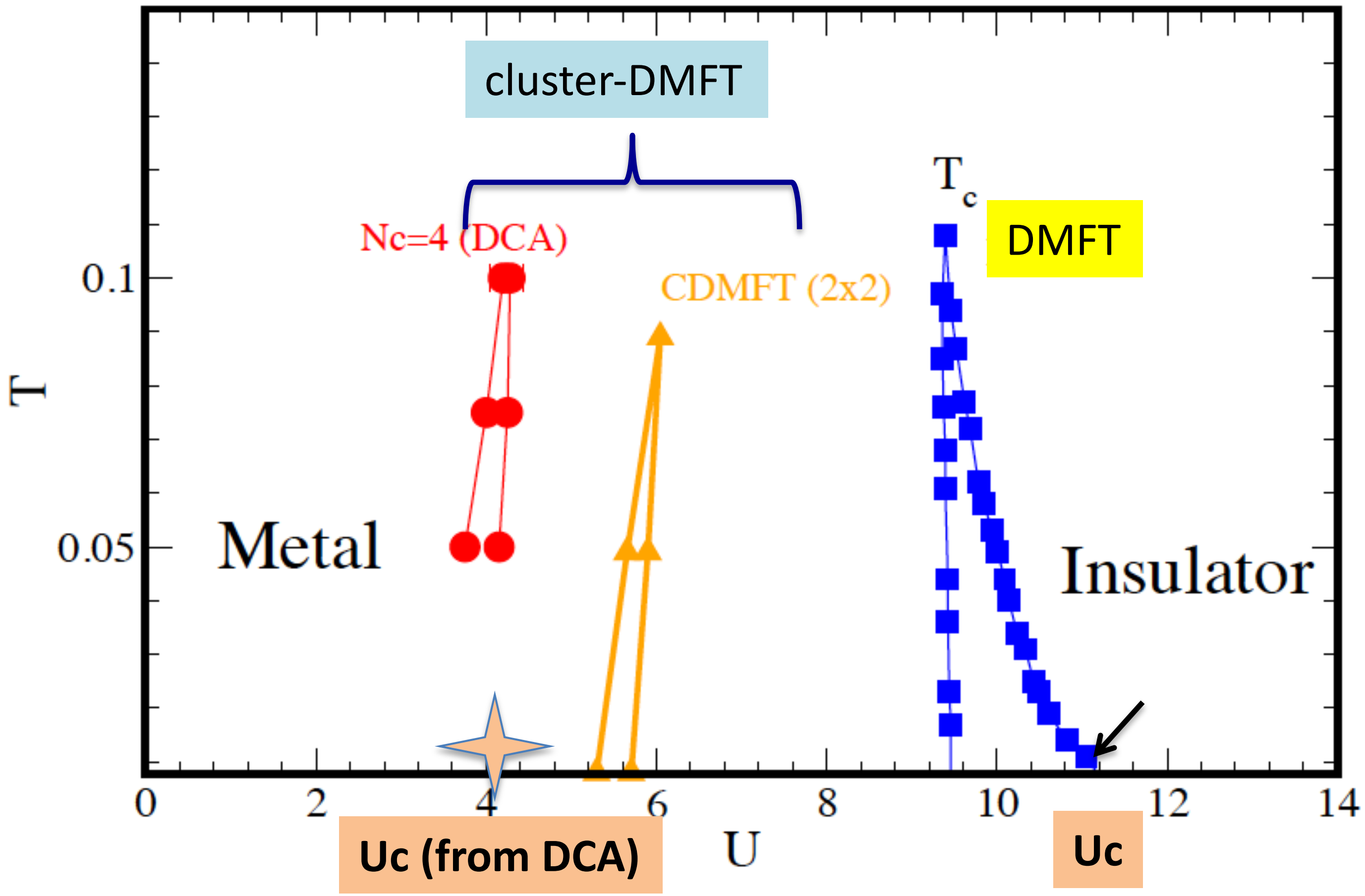
- Nonlocal physics at low T will be lattice dependent and calls for experiments on lattices beyond triangular lattices.

- And computation beyond DMFT and different lattices.

Recent Advances

Theory prospective: beyond local DMFT

$$H = -\sum_{<ij,\sigma>} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



DMFT; Georges et al., Rev. Mod. Phys. 68, 13 (1996)

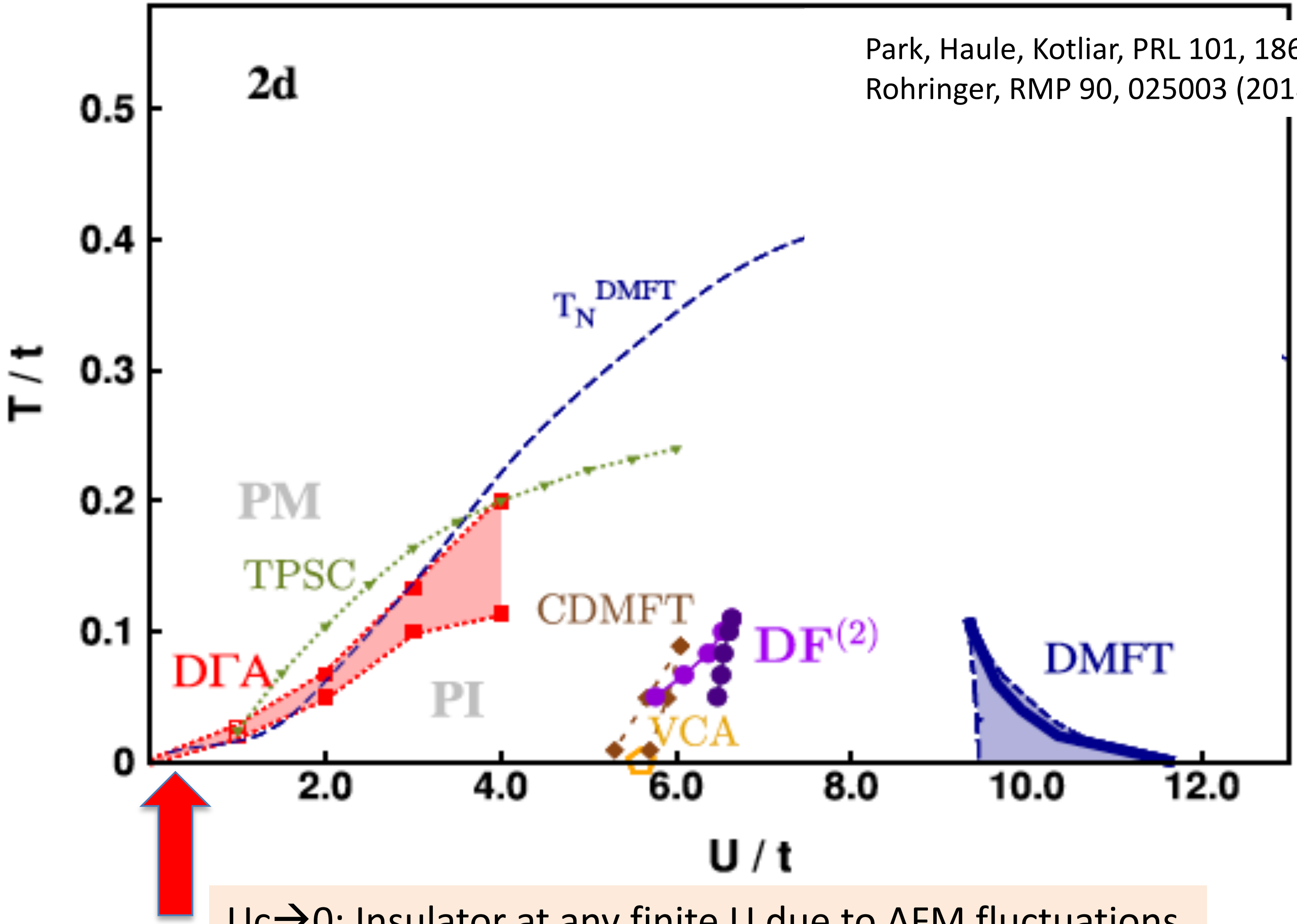
T. Maier, Quantum cluster theorties, RMP, 2005.

Park, Haule, Kotliar, PRL 101, 186403 (2008).

Uc for MIT gets suppressed beyond DMFT level: non-local correlations are important

Fate of Mott transition in 2D

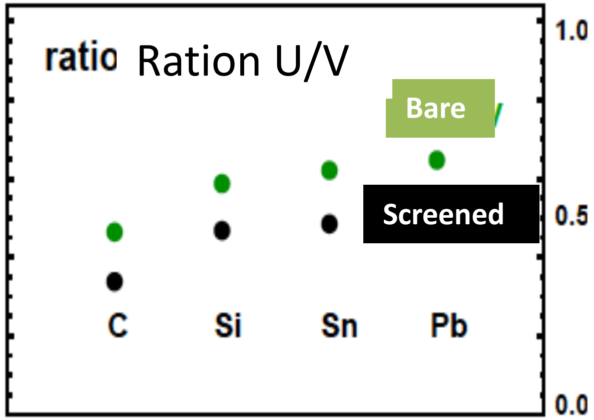
Park, Haule, Kotliar, PRL 101, 186403 (2008).
Rohringer, RMP 90, 025003 (2018).

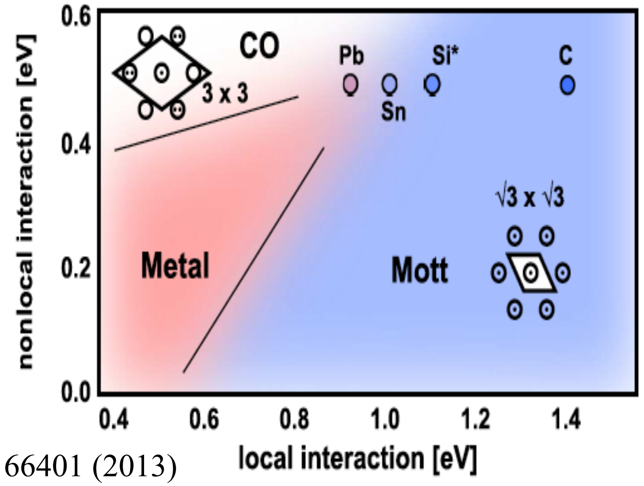


Uc→0: Insulator at any finite U due to AFM fluctuations

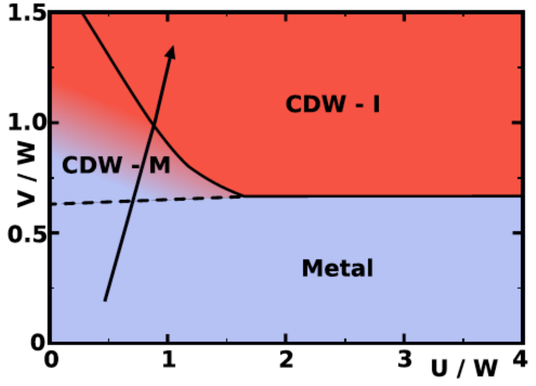
Beyond Hubbard model: Non-local Coulomb interactions effects in realistic materials

Adatom





from Hansmann et al., Phys. Rev. Lett. 110, 166401 (2013)



Nature Physics, 4, 932 (2008)

- **Calculations <u>show sizable non-local interactions</u> in:**
  Adatoms on semiconducting surface Si:X (X=Sn, C, Si, Pb)
  Nonlocal V reaches ~30~60% U
  (PRL 110, 166401, 2013)

- **<u>Strong screening</u>** in graphene , benzene, silicine
  - **nonlocal interactions are found to reduce local one by a factor of two**
  (PRL 111, 036601, 2013)

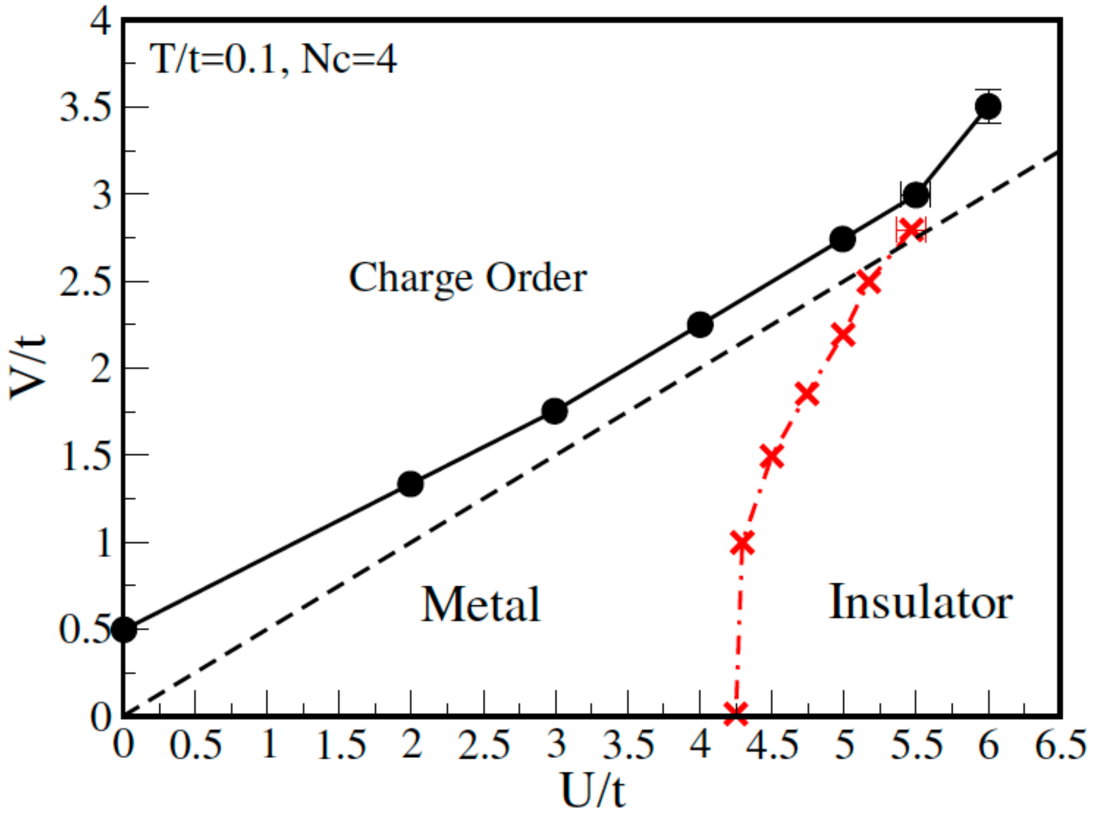
- **Charge ordering**
  -Wigner-Mott transitions;

Our focus: can non-local interactions V stabilize the MIT in 2D?

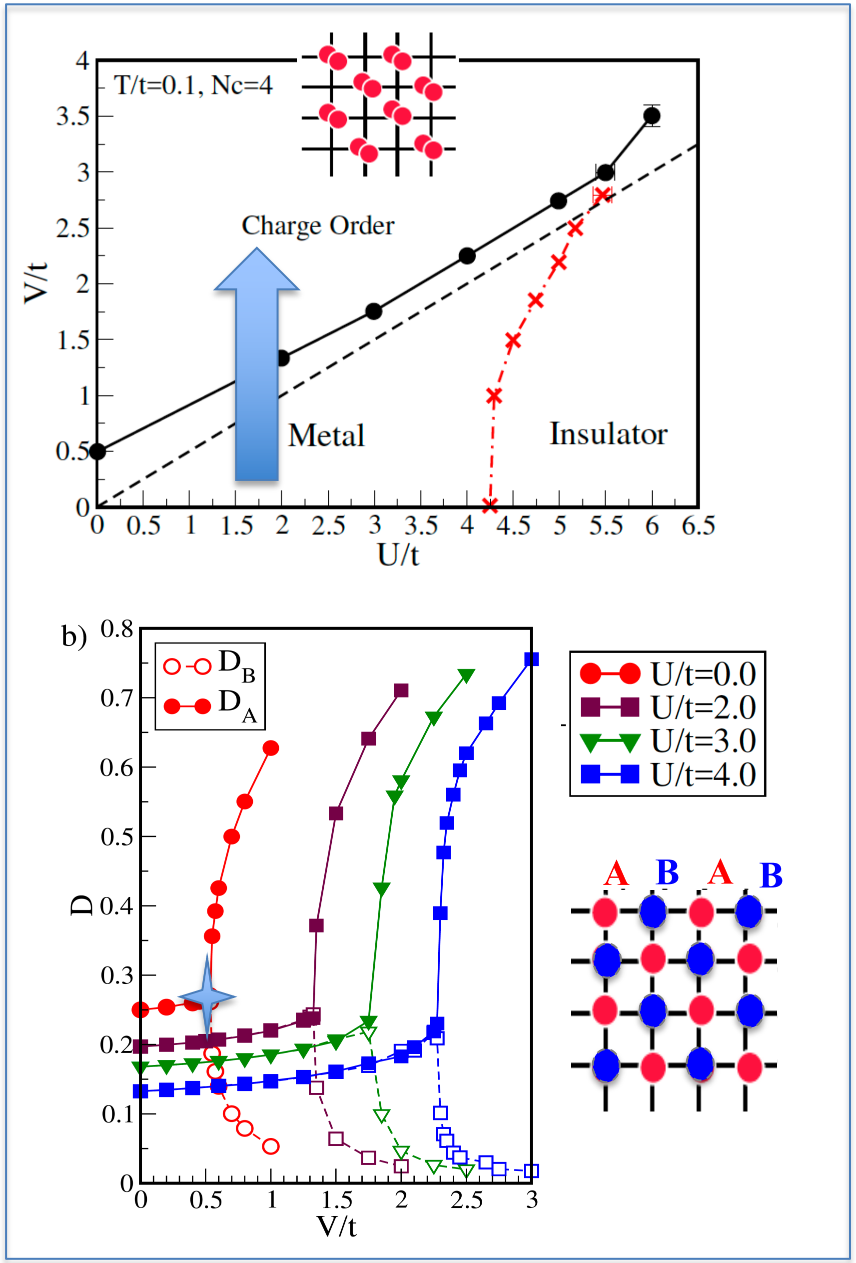
Extended Hubbard Model

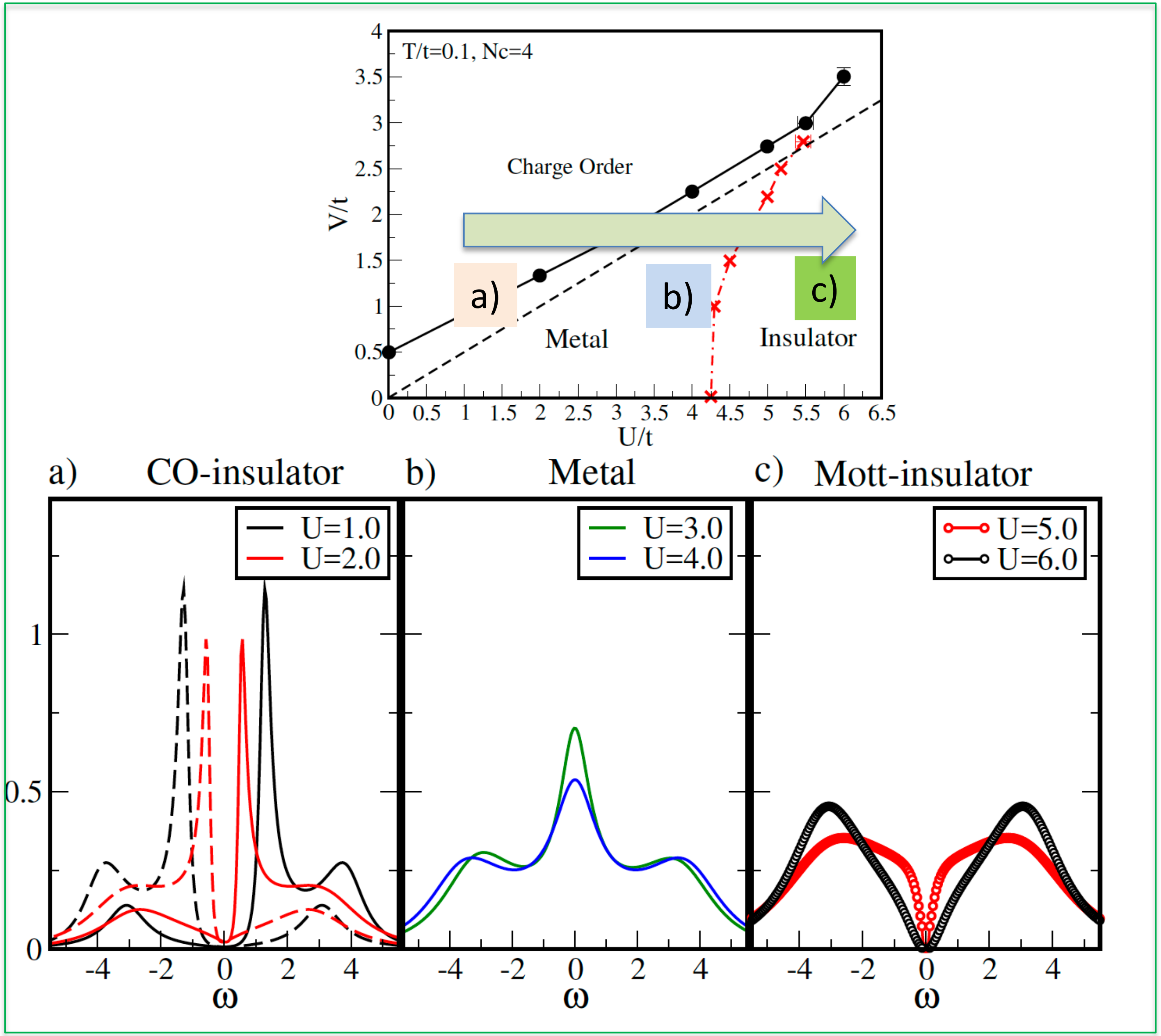
EHM: the competition between onsite U and inter-site V interaction; The minimal model for charge order:

$$H = -\sum_{<ij;\sigma>} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + \frac{V}{2}\sum_{<ij>;\sigma\sigma'} n_{i\sigma}n_{j\sigma'}$$

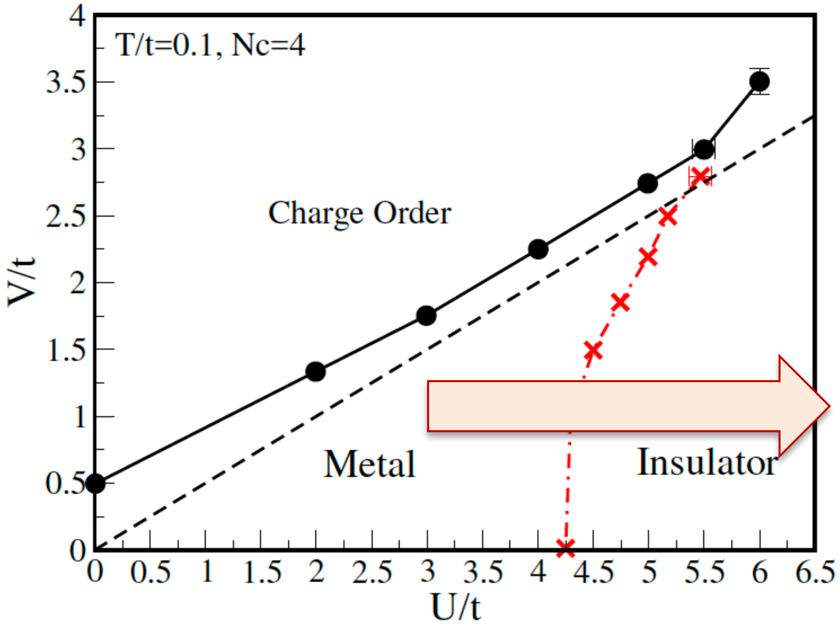


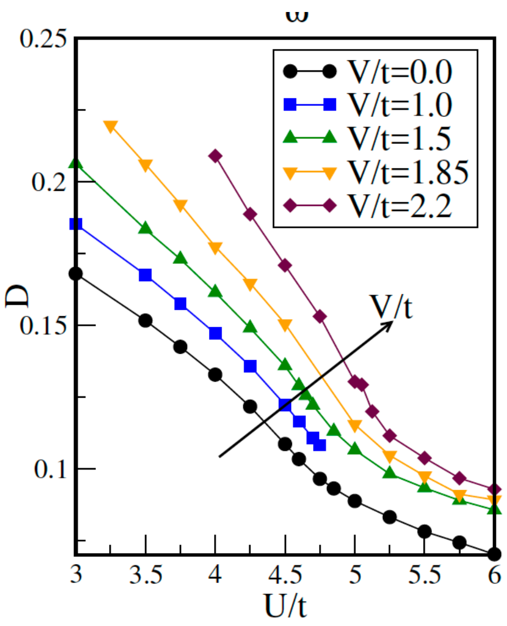
Extended Hubbard Model

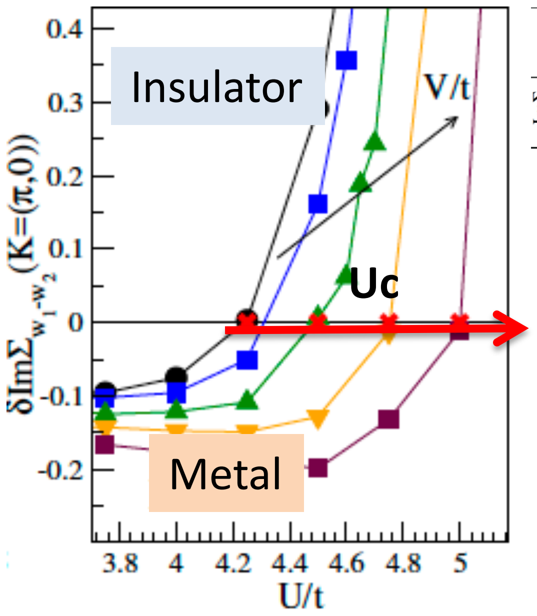


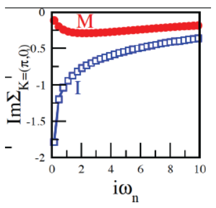


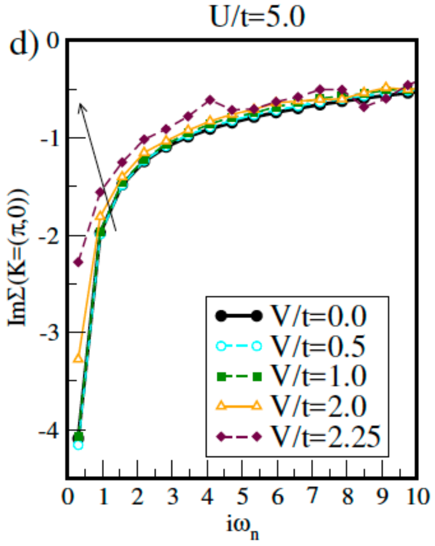
V effect on Mott insulating behavior

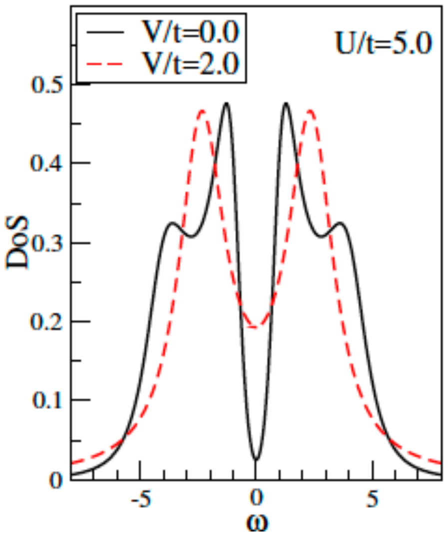












Nonlocal inter-site interactions V push the metal-insulator transition boundary to a larger U values due to screening effects. **This indicates possible stabilization of MIT in 2D Hubbard model at large clusters.**

V suppresses self-energy, making system less insulating due to screening effects.

Conclusion

- DMFT reveals QC scaling of resistivity in high temperature regime.
- Four different experimental groups confirmed such scaling. High temperature Mott Quantum Critical crossover a **ubiquitous universal feature of various types of Mott transitions.**
- In 2D square Hubbard model the non-local correlations beyond DMFT level are important; they suppresses the coexistence region and significantly reduce the critical U value at which transition happens.
- Some beyond Hubbard perturbations: finite V, the metal-insulator boundary is pushed to a larger U values, suggesting that non-local inter-site interactions V might possibly stabilize the MIT in 2D.

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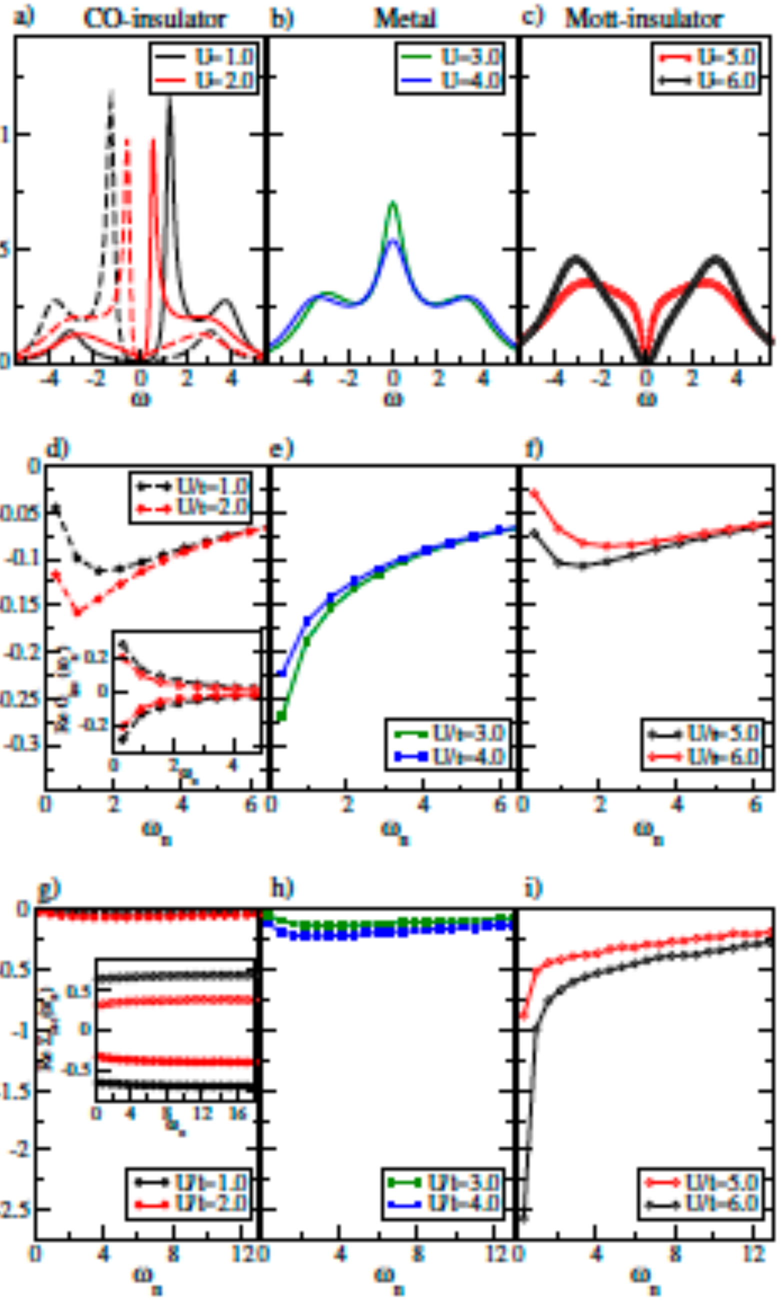
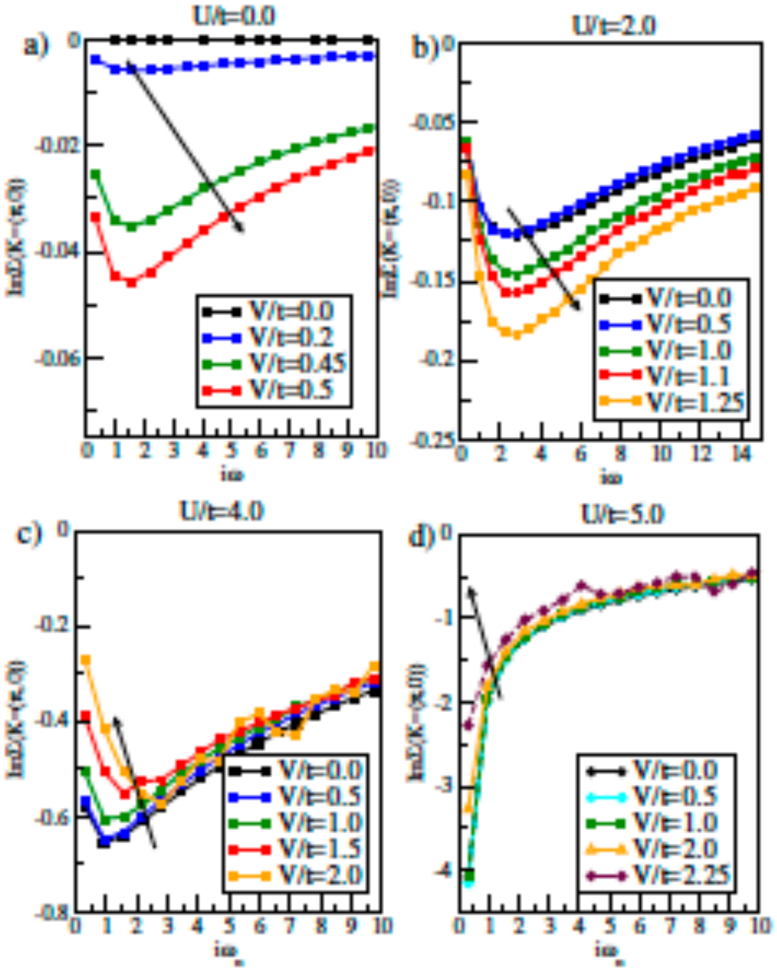

a) CO-insulator
b) Metal
c) Mott-insulator
U=1.0
U=2.0
U=3.0
U=4.0
U=5.0
U=6.0
DOS
ω
d)
e)
f)
U/t=1.0
U/t=2.0
U/t=3.0
U/t=4.0
U/t=5.0
U/t=6.0
Im G$_{loc}$(ω$_n$)
ω$_n$
g)
h)
i)
Im Σ$_{loc}$(ω$_n$)


U/t=0.0
U/t=2.0
U/t=4.0
U/t=5.0
a)
b)
c)
d)
V/t=0.0
V/t=0.2
V/t=0.45
V/t=0.5
V/t=0.5
V/t=1.0
V/t=1.1
V/t=1.25
V/t=1.5
V/t=2.0
V/t=2.25
ImΣ(K=(π,0))
iω
iω$_n$