Superconductivity in quasi-2d organic doped Mott insulators: a superconducting dome without an antiferromagnetic quantum critical point

C.-D. Hébert, P. Sémon,

A.-M. Tremblay

C.-D. Hébert, P. Sémon, A.-M.S. Tremblay PRB **92**, 195112 (2015)

APS Baltimore, R25.13 Superconductivity Less Common Materials I

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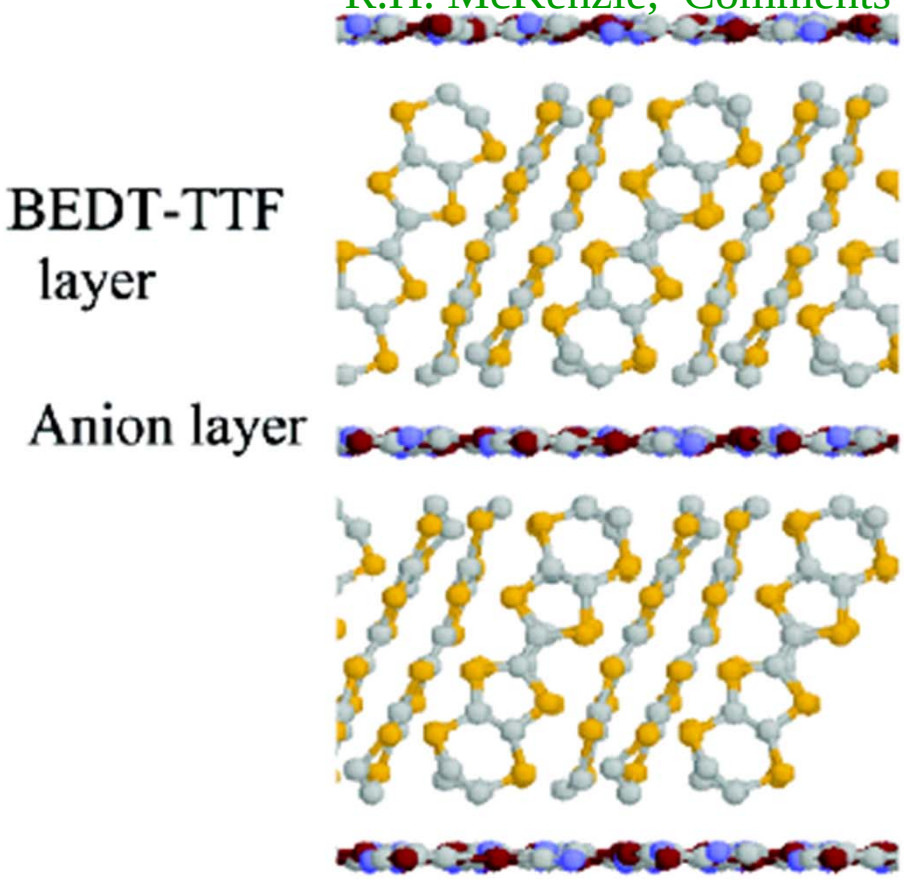
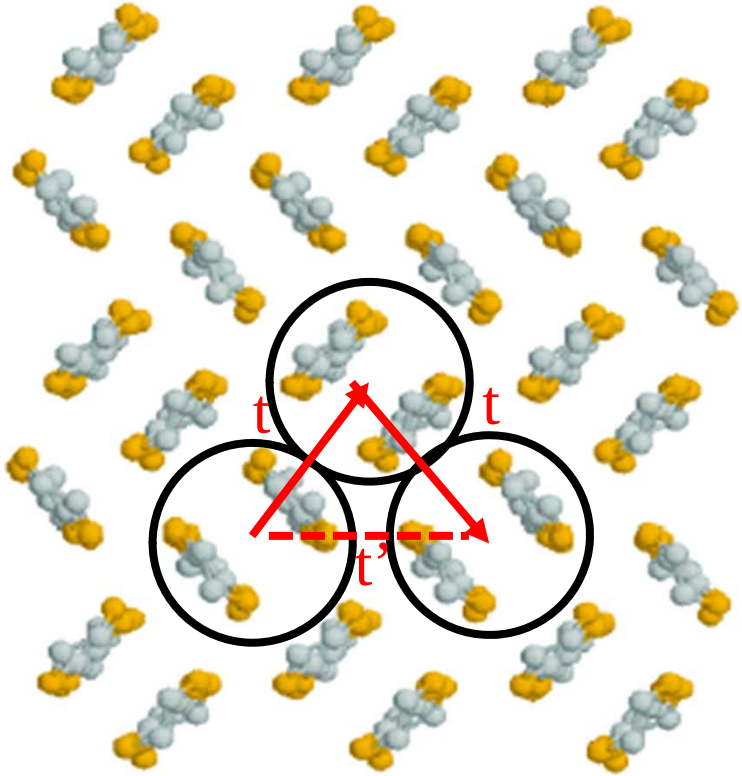
Layered organics (κ–BEDT-X family)

H. Kino + H. Fukuyama, J. Phys. Soc. Jpn **65** 2158 (1996),
R.H. McKenzie, Comments Condens Mat Phys. **18**, 309 (1998)





$t \approx 50\ \text{meV}$

$\Rightarrow U \approx 400\ \text{meV}$

$t'/t \sim 0.6 - 1.1$

Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

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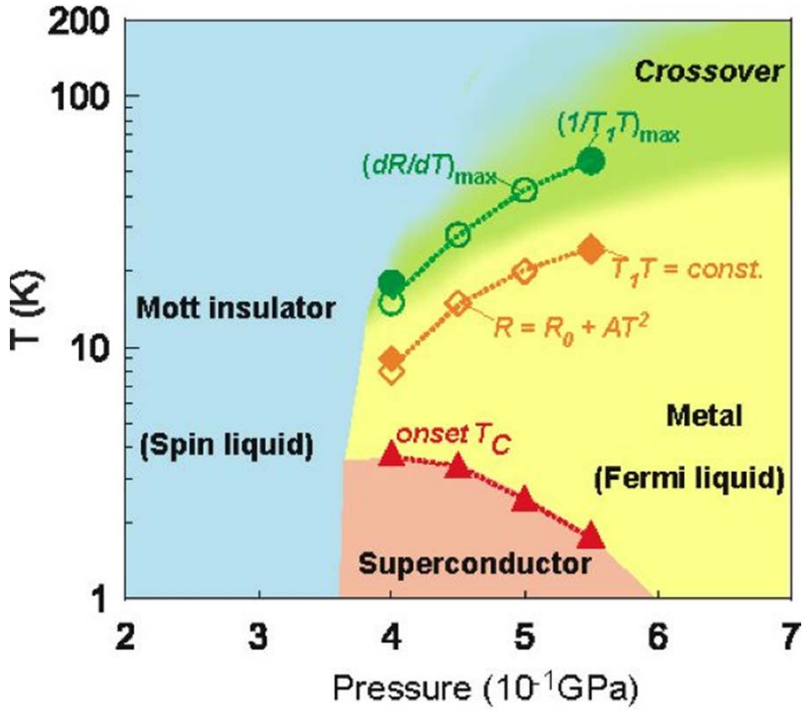
Phase diagram at $n = 1$

$X = Cu_2(CN)_3$ $(t' \sim t)$



Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

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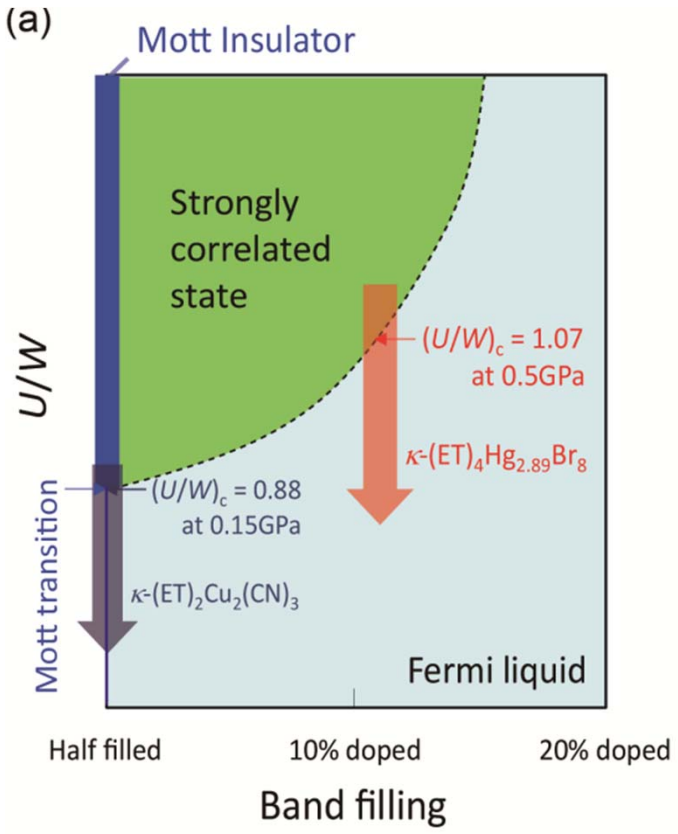
A doped BEDT organic



	W (eV)	U (eV)	U/W	BF	T_c (K)
κ-$Cu(NCS)_2$ [a)]	0.57	0.46	0.81	0.50	10.4
κ-$Cu[N(CN)_2]Br$ [a)]	0.55	0.49	0.89	0.50	11.8
κ-$Hg_{2.89}Br_8$ [b)]	0.26	0.465	1.79	0.45	4.3

H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Taniguchi et al. J. Phys. Soc. Japan, **76**, 113709 (2007)

R. N. Lyubovskaya et al. JETP Lett. **45,** 530 (1987)

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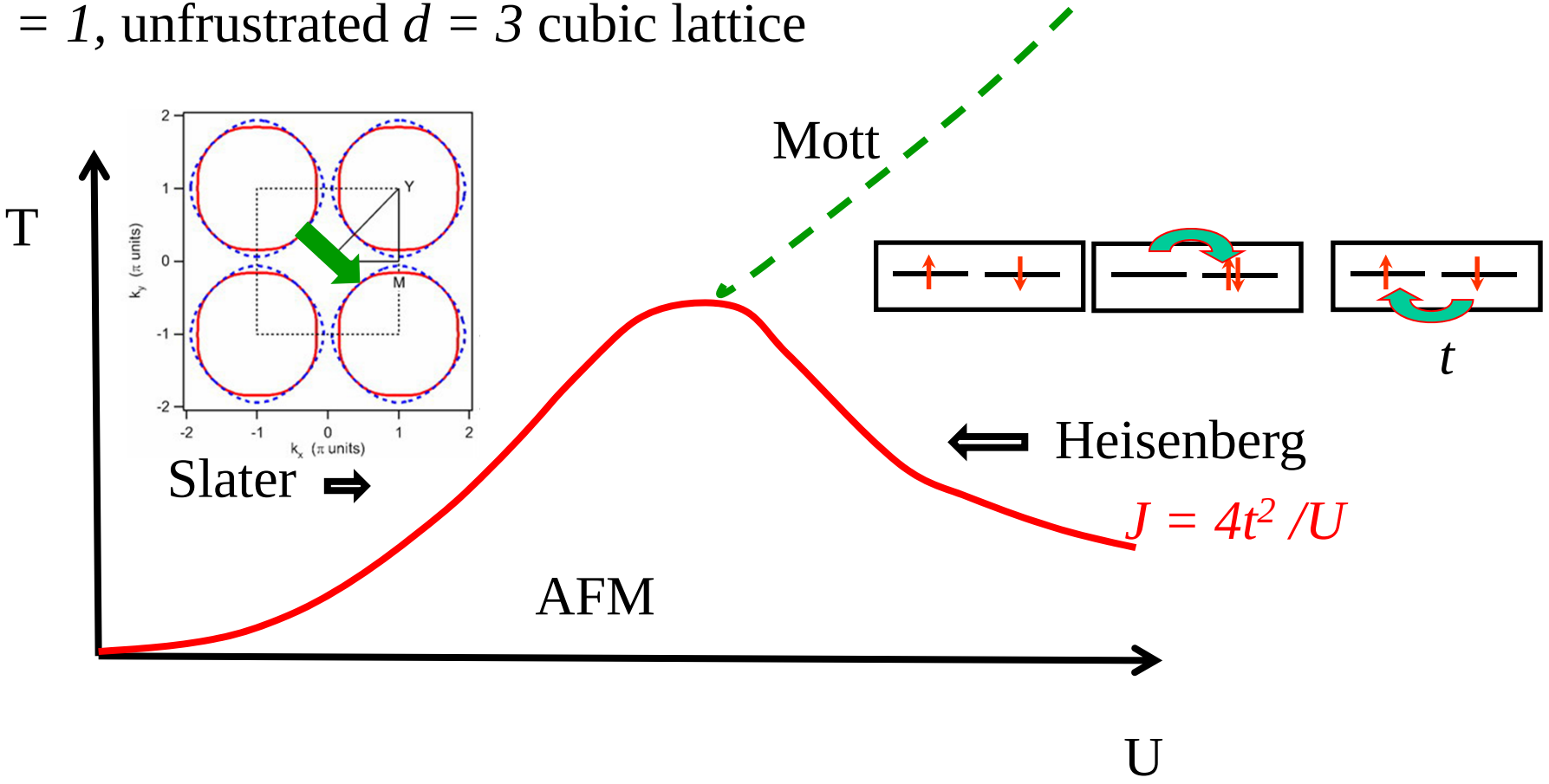
Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

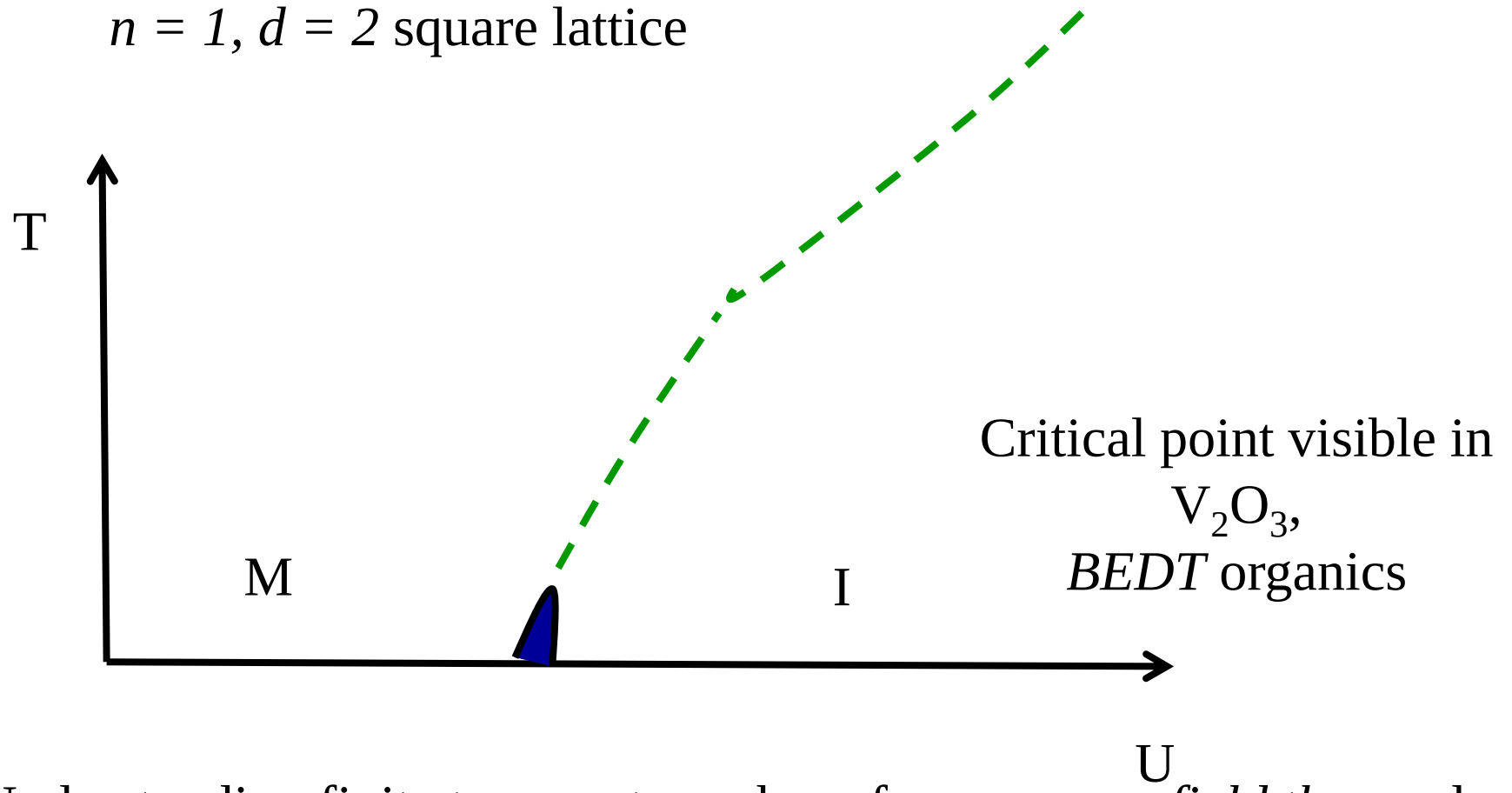
Weak vs Strong correlations

n = 1, unfrustrated *d = 3* cubic lattice



Local moment and Mott transition

n = 1, d = 2 square lattice



Understanding finite temperature phase from a *mean-field theory* down to *T = 0*

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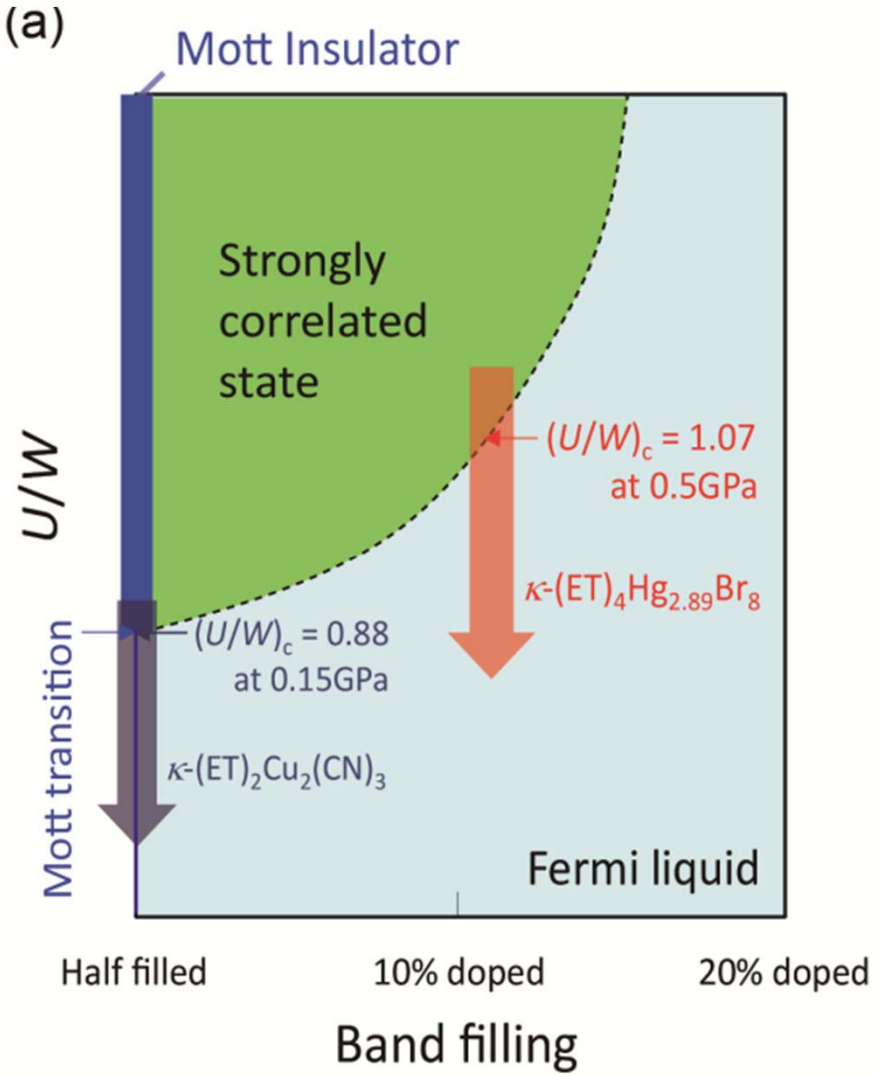
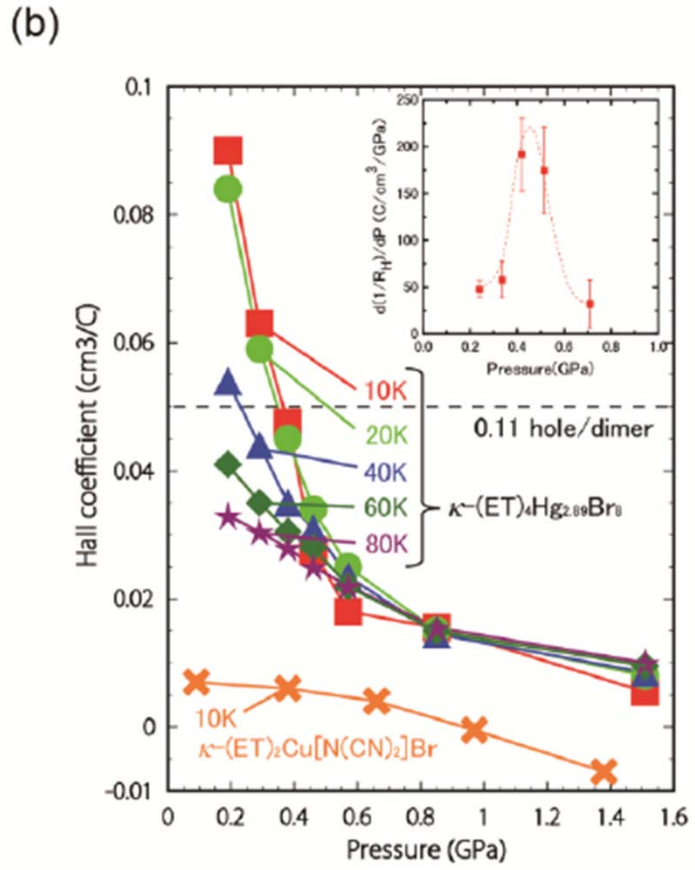
Doped organic: experiment

Doped BEDT





H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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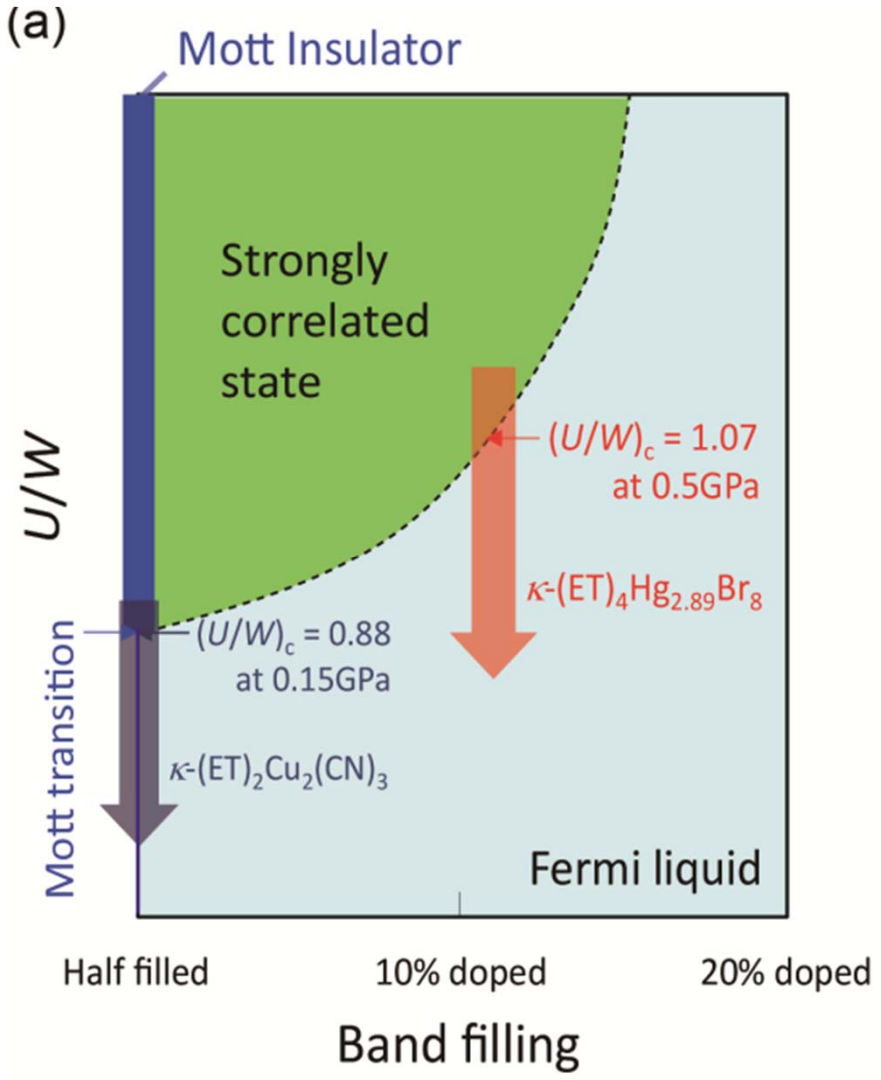
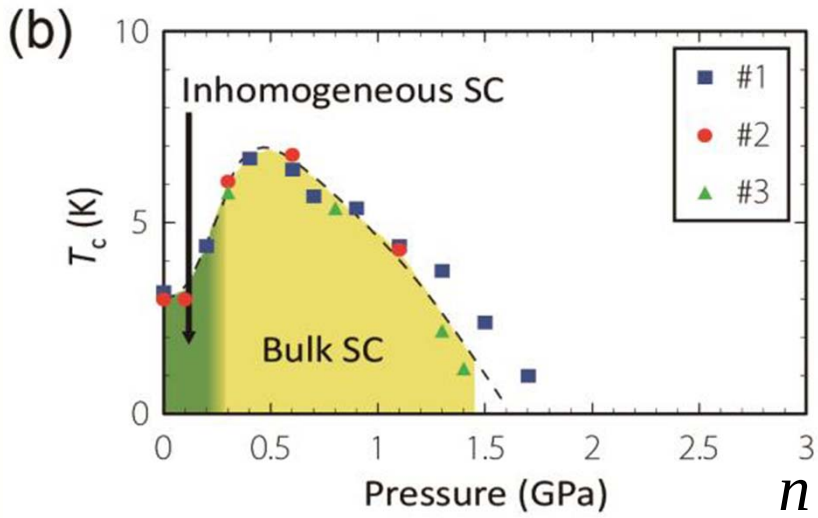
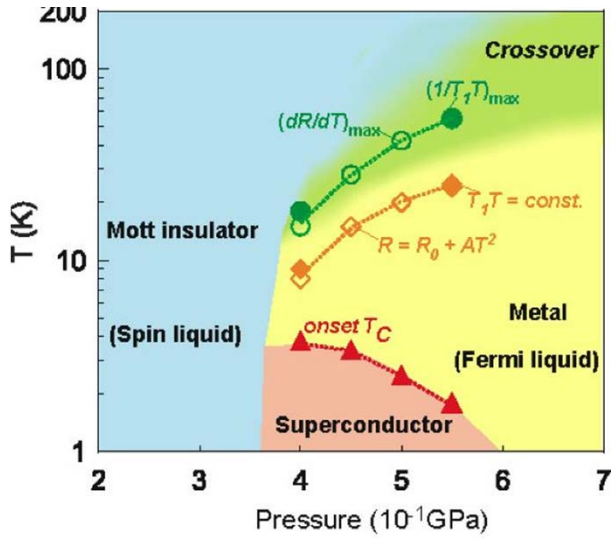
Doped BEDT





n = 0.90



n= 1

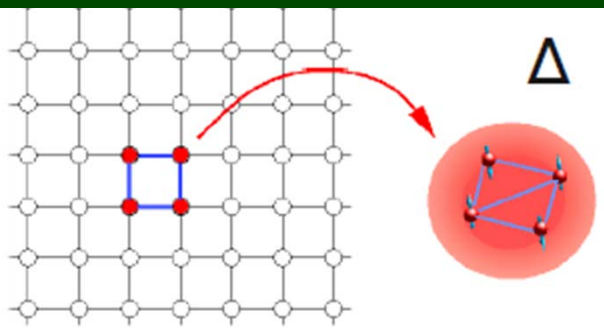
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Method

Concept: Cluster - DMFT

Tools: Impurity solver

CTQMC impurity solver (tool) (*T* finite)

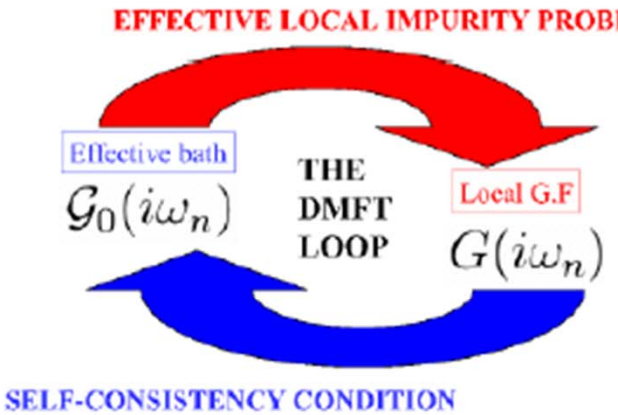


$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau)\Delta_{\mathbf{K}}(\tau,\tau')\psi_{\mathbf{K}}(\tau')}$$

Mean-field is not a trivial problem! Many impurity solvers.

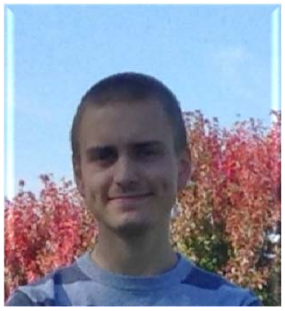
Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007



$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

P. Sémon *et al.*
PRB **85**, 201101(R) (2012)
PRB **90** 075149 (2014);
and PRB **89**, 165113 (2014)



Charles-David Hébert

Patrick Sémon

Organics : Phase diagram, finite T

Made possible by algorithmic improvements

P. Sémon *et al.*
PRB **85**, 201101(R) (2012)
PRB **90** 075149 (2014);
and PRB **89**, 165113 (2014)

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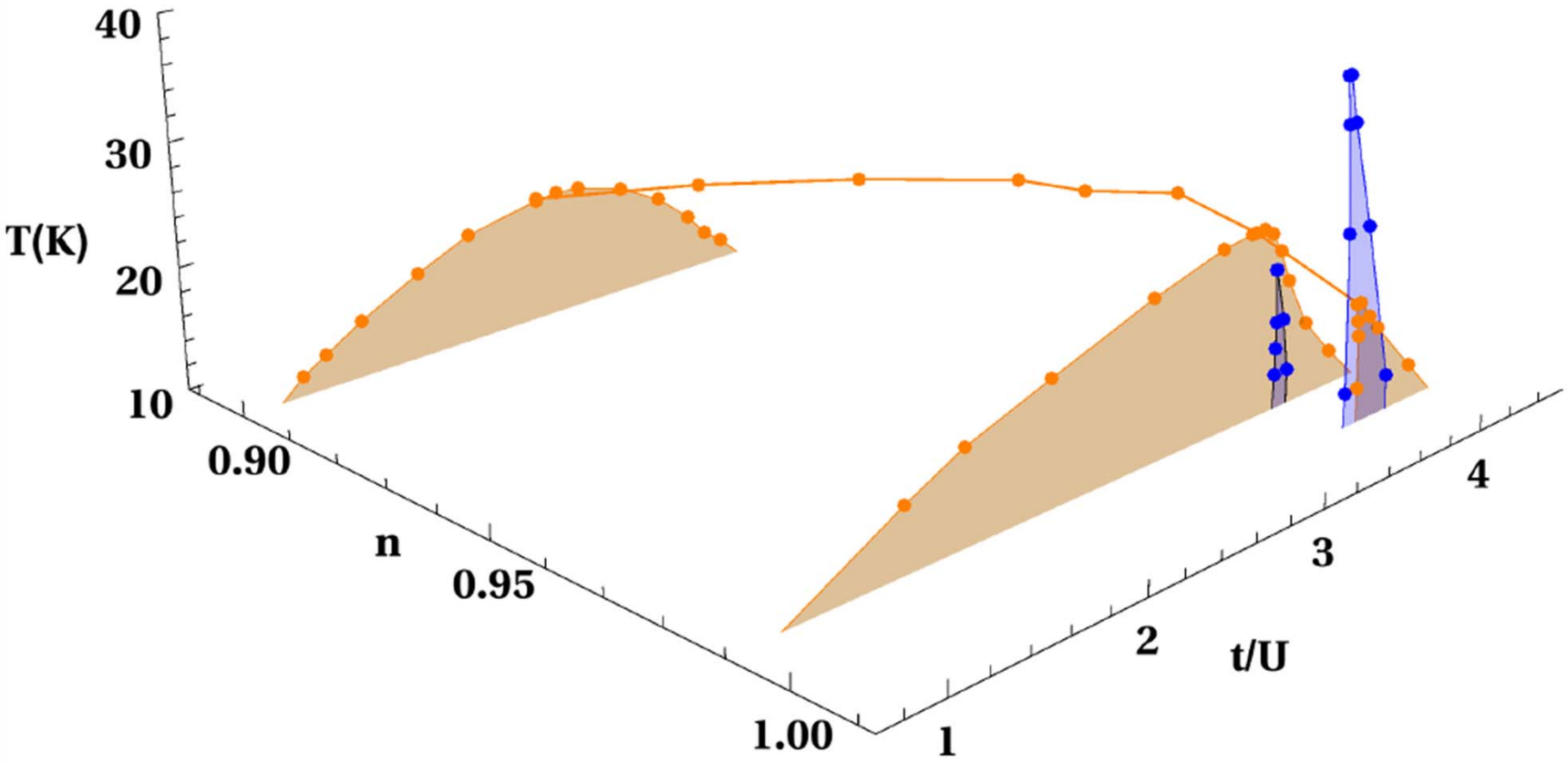
$t' = 0.4t$ overview



Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

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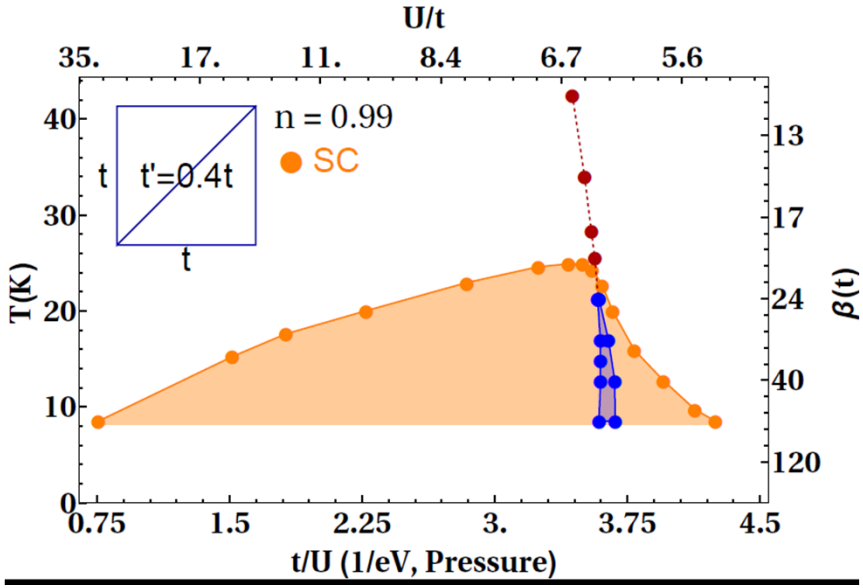
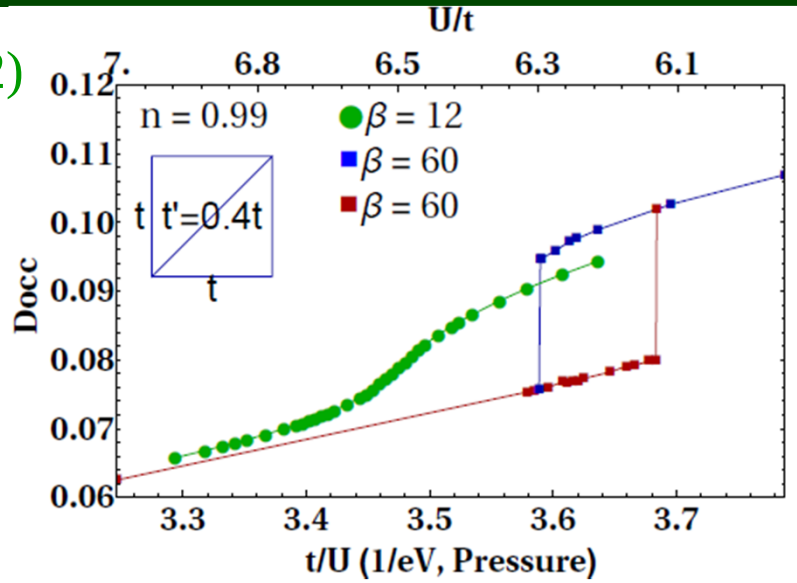
First order and Widom line in organics

G. Sordi *et al.* Scientific Reports, **2**, 547 (2012)





Compare: T. Watanabe, H. Yokoyama and M. Ogata JPS Conf. Proc. **3**, 013004 (2014)

C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

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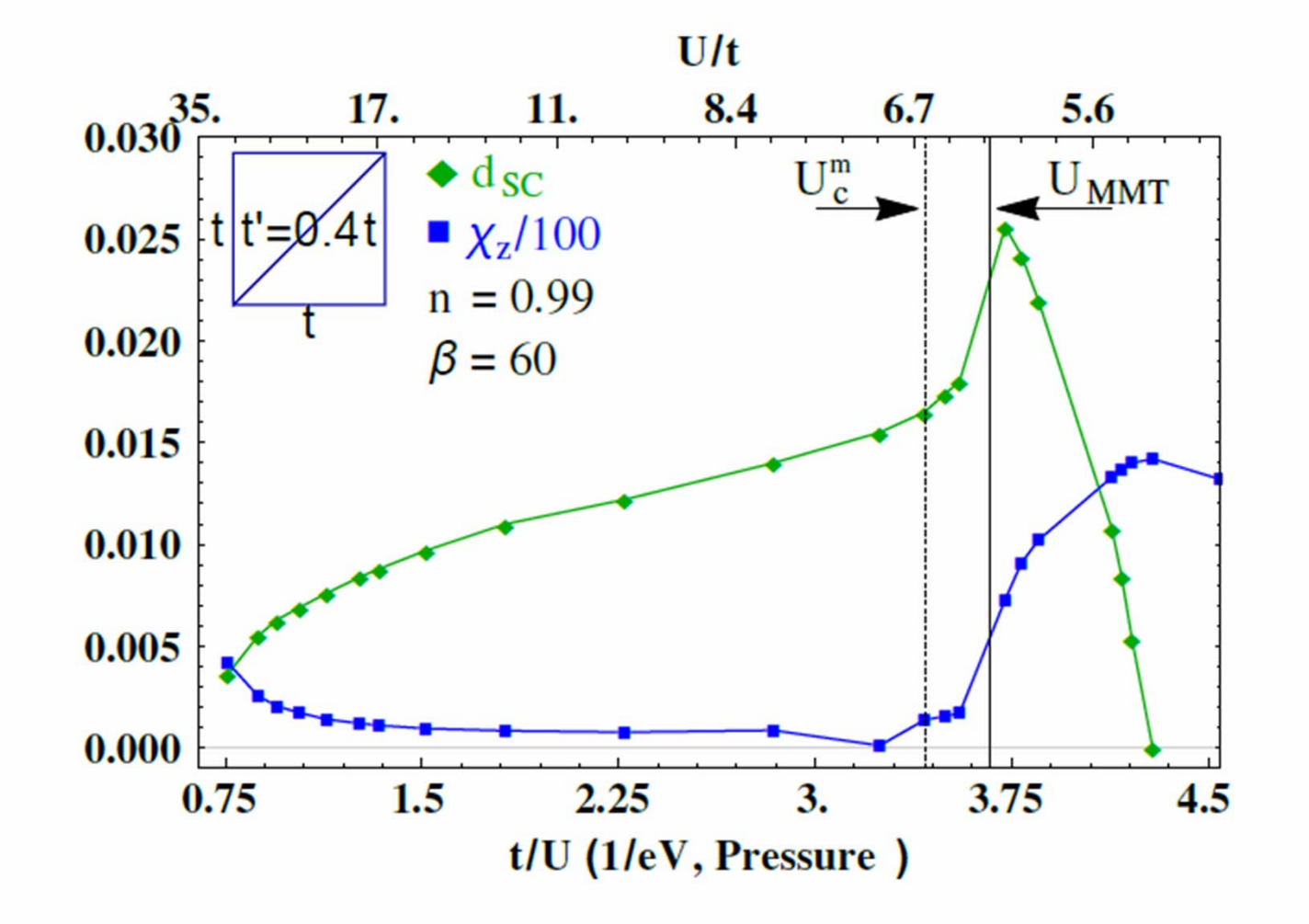
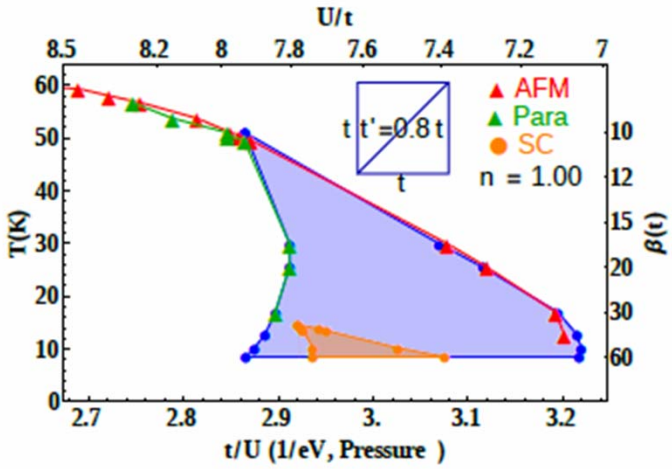
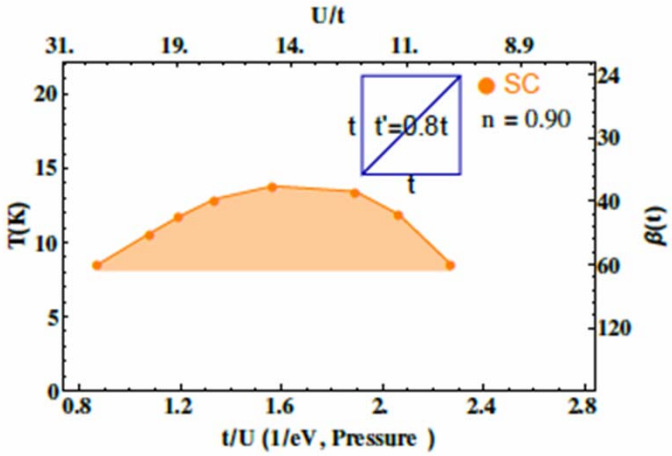
Signatures of Widom line in the superconducting state



$t' = 0.8\ t$



(a)



(b)

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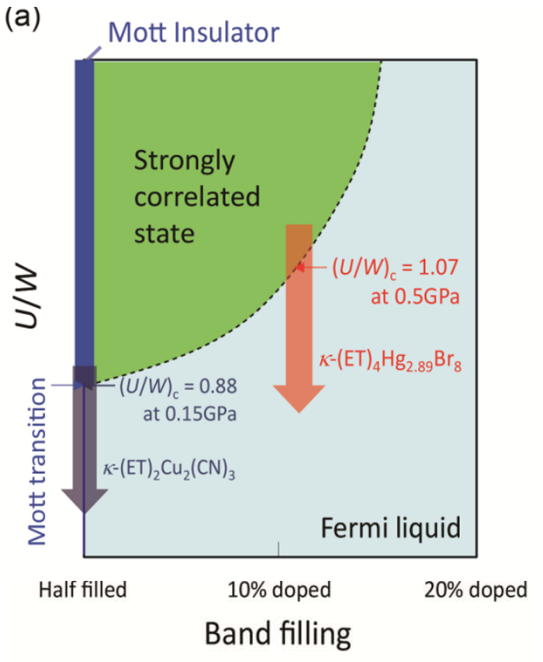
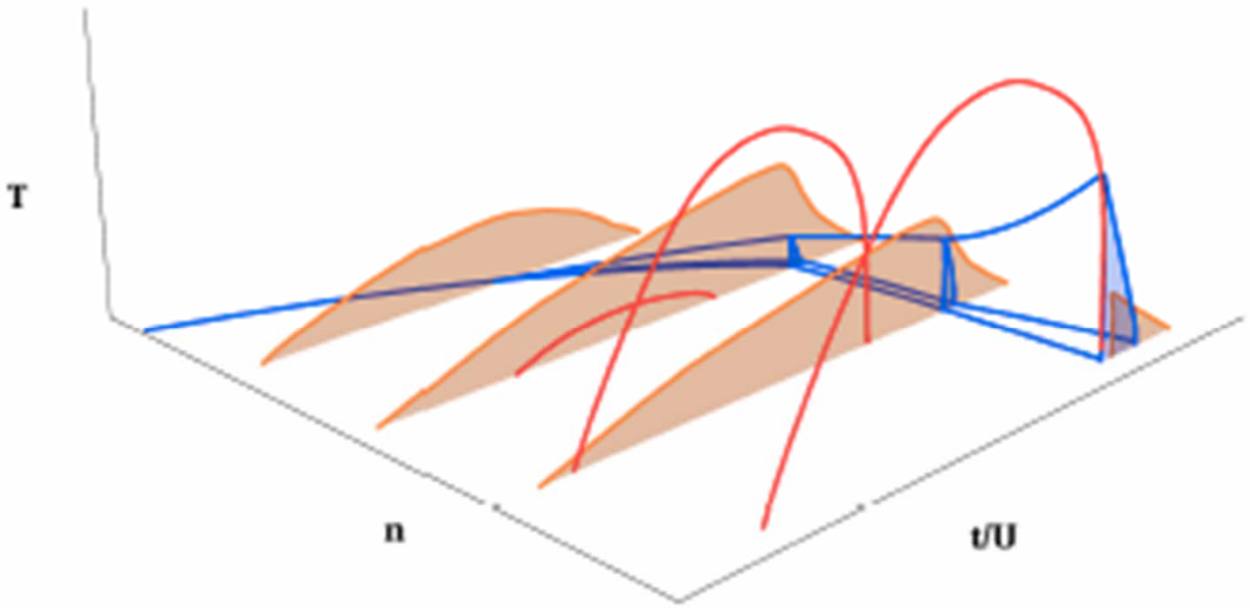
Generic case highly frustrated case





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Wei Wu

AFM quantum critical point in heavy fermions (with same category of methods)

W. Wu A.-M.S.T. Phys. Rev. X, 2015

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Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N *much more* than T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state
  - or remnants in SC state
  - also T_c decreases in e-doped
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c dome maximum near normal state 1st order

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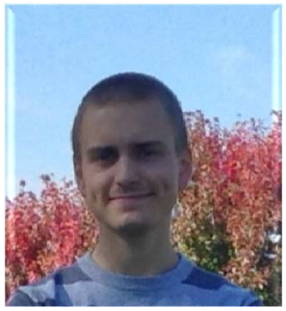
Collaborators for this work



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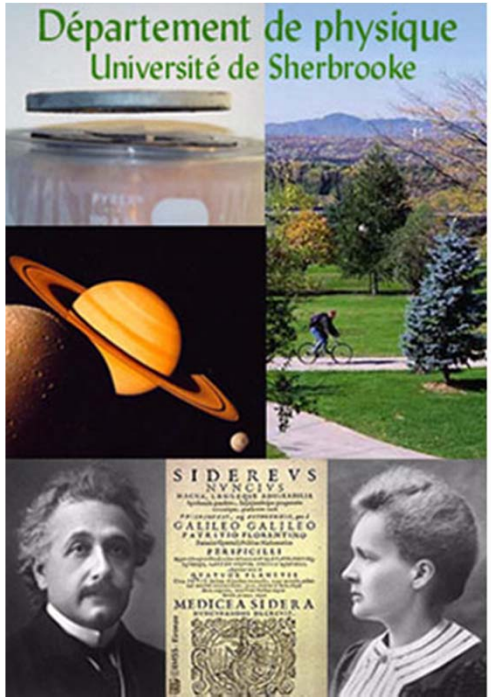

André-Marie Tremblay

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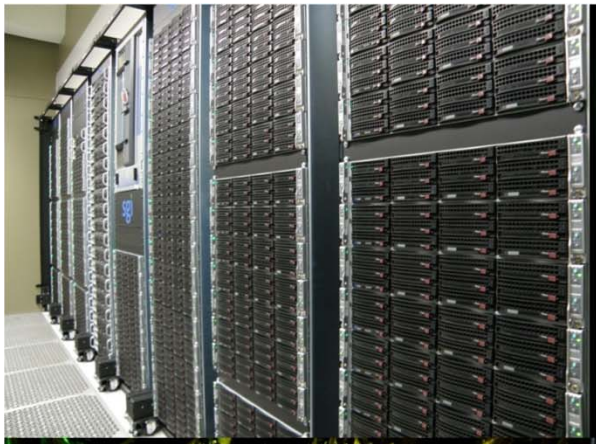

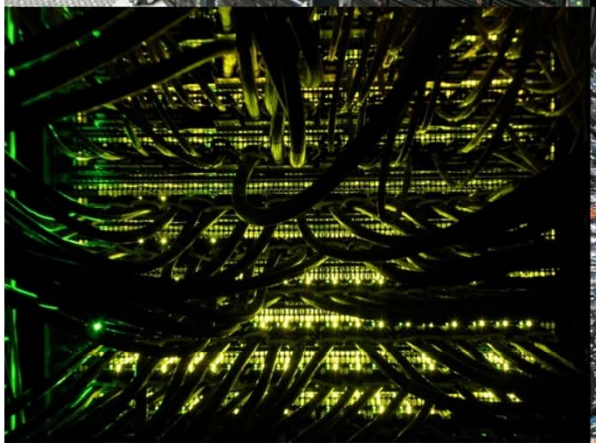

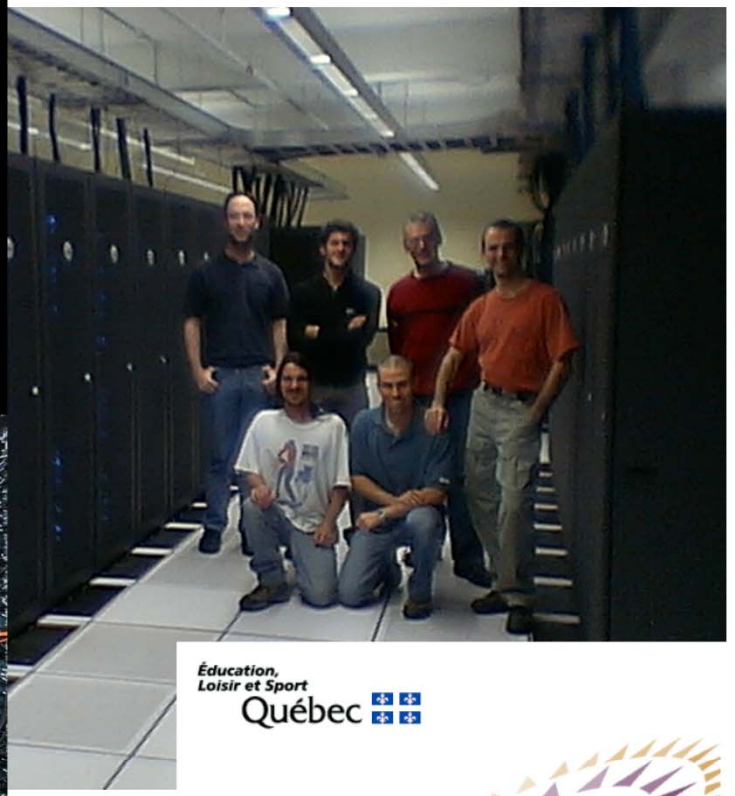

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Review: A.-M.S.T. arXiv: 1310.1481

A.-M.S. Tremblay

"Strongly correlated superconductivity"

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation, Vol. 3*, E. Pavarini, E. Koch, and U. Schollwöck (eds.)

Verlag des Forschungszentrum Jülich, 2013