A unified perspective on cuprates and layered organic superconductors

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M2S Geneva, 28 August 2015

VERITATEM IN CHARITATE

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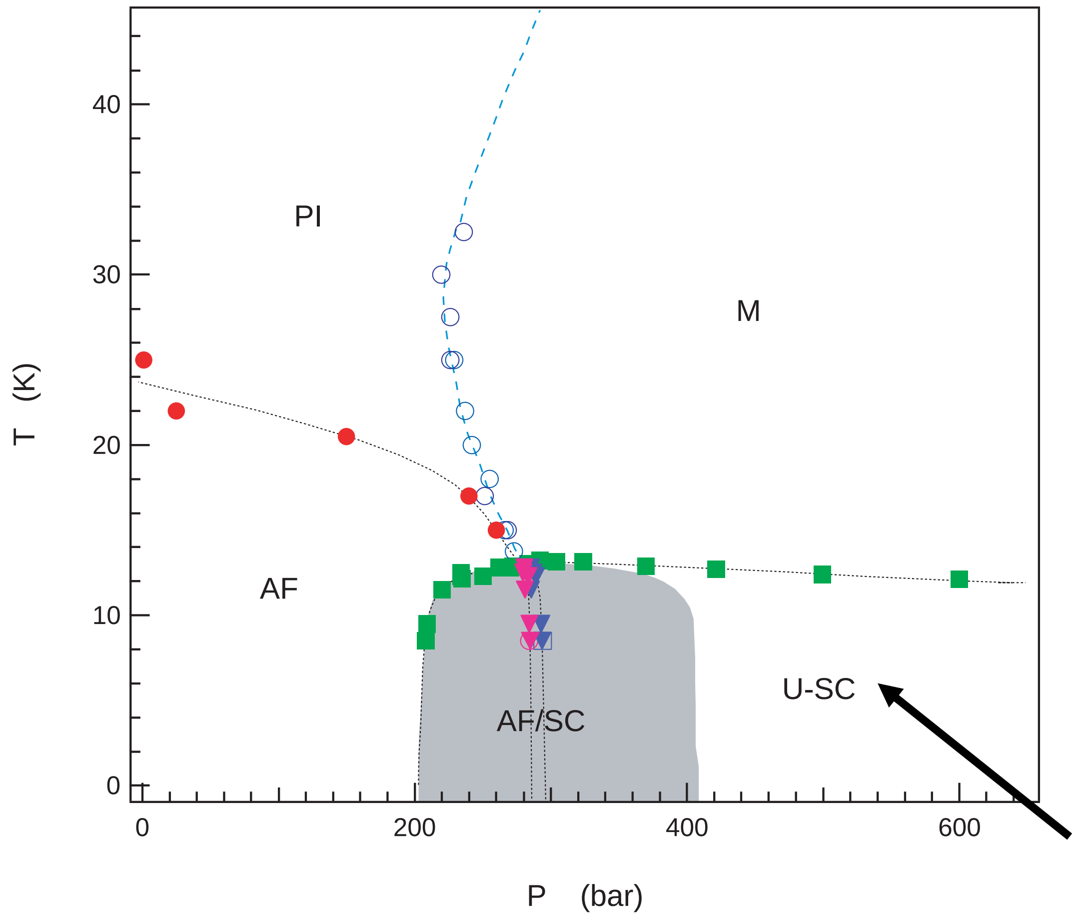
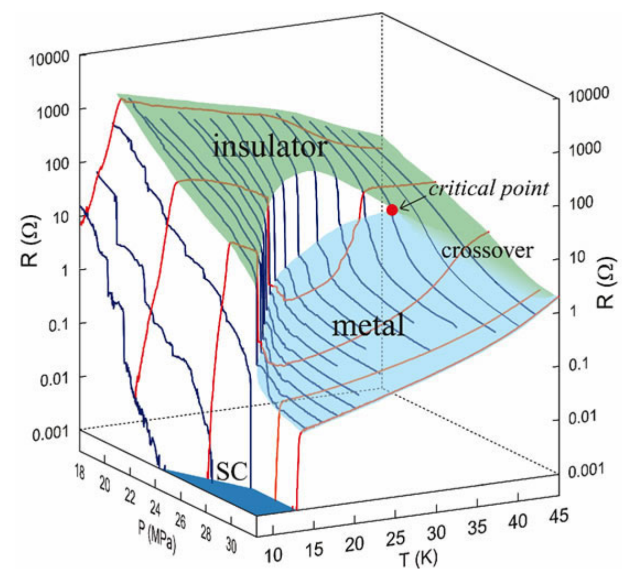
Phase diagram for organics





F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

B_g for C_{2h} and B_{2g} for D_{2h}

Powell, McKenzie cond-mat/0607078

Phase diagram (X=Cu[N(CN)$_2$]Cl)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

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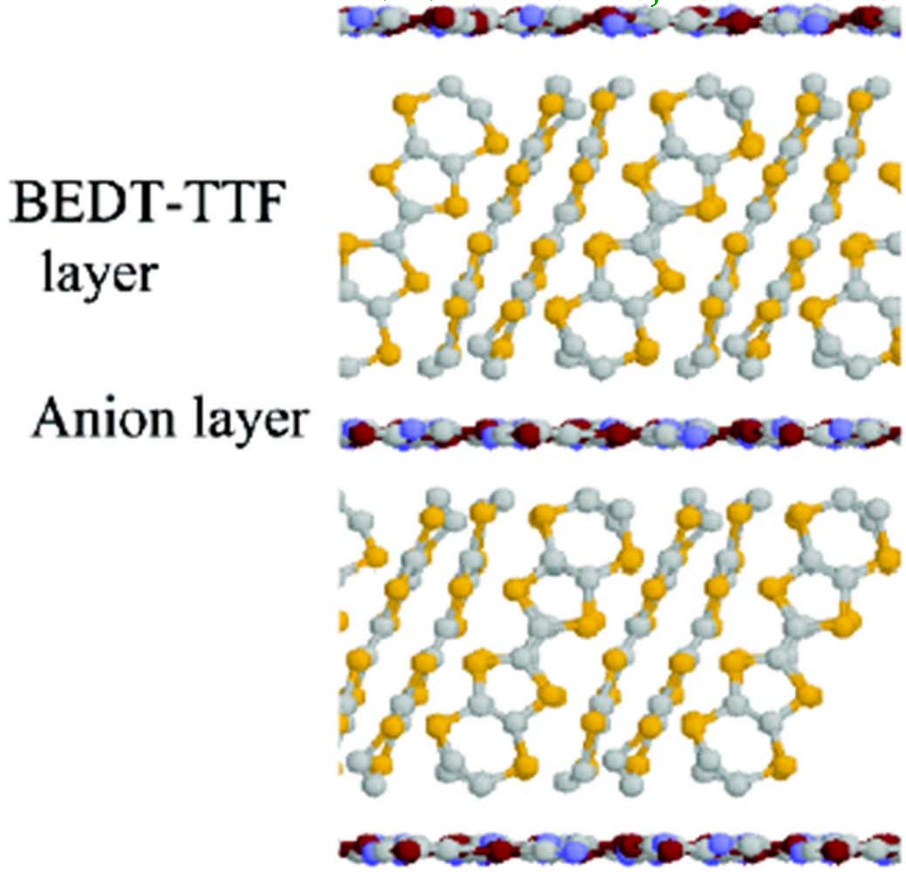
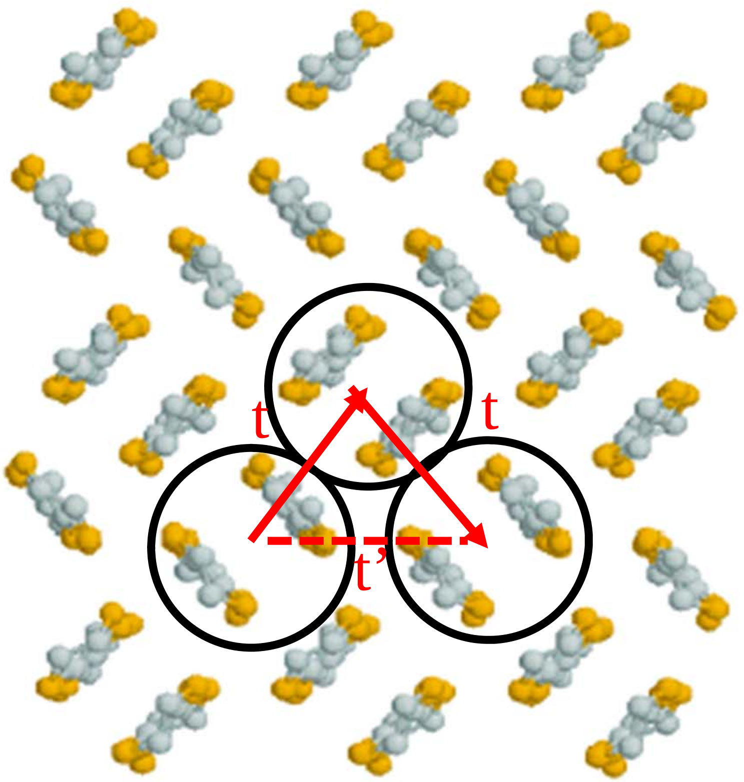
Layered organics (κ–BEDT-X family)

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





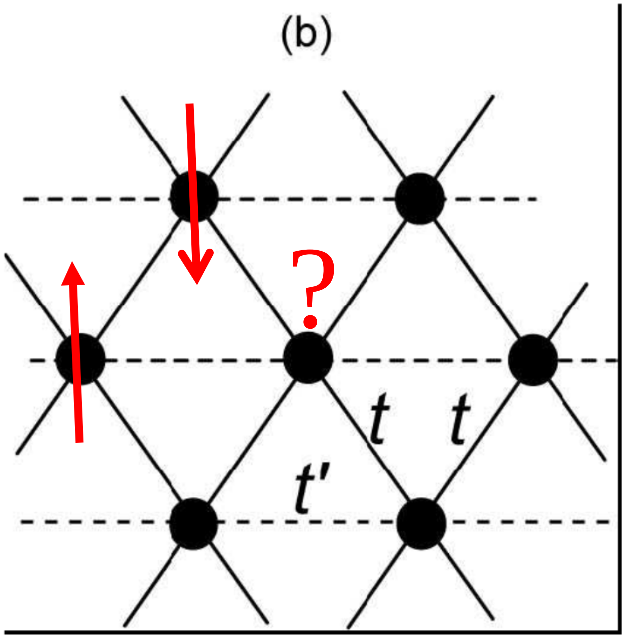
Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)

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

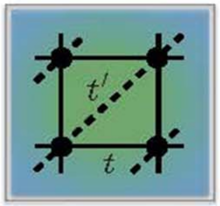
$$\Rightarrow U \approx 400\,\text{meV}$$

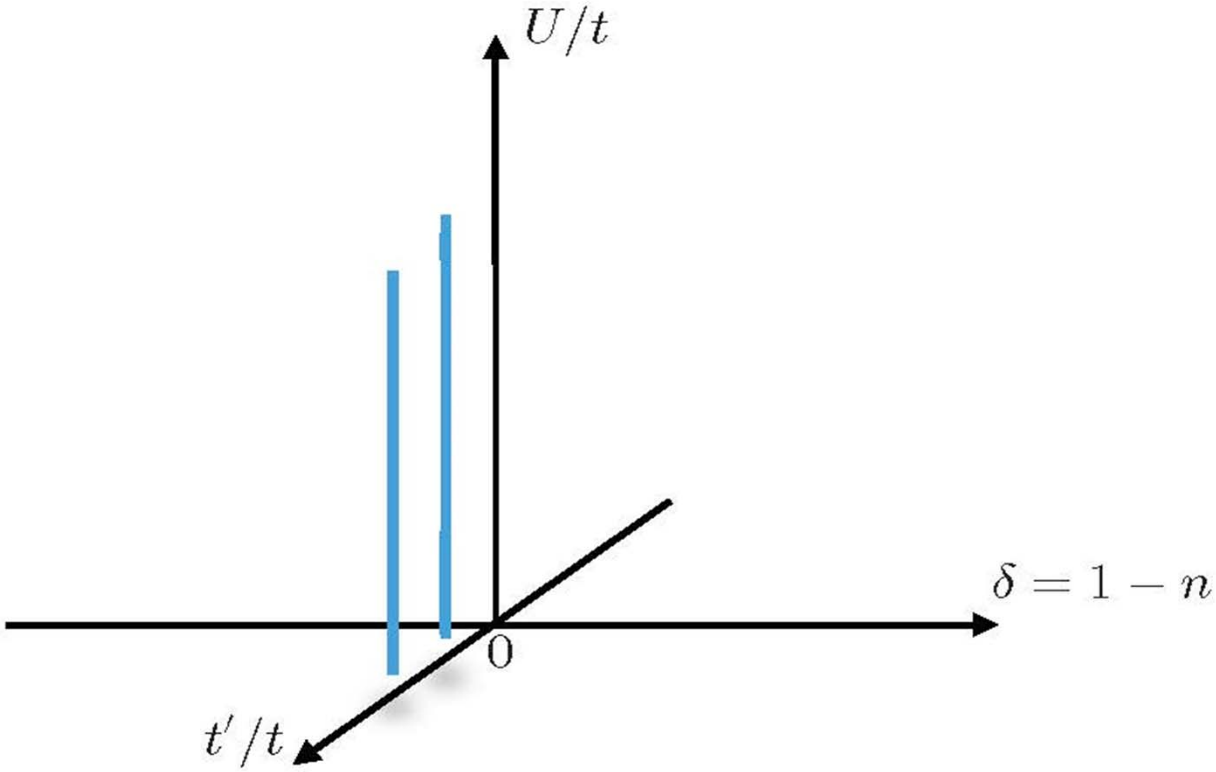
$$t'/t \sim 0.6 - 1.1$$

Magnetic frustration

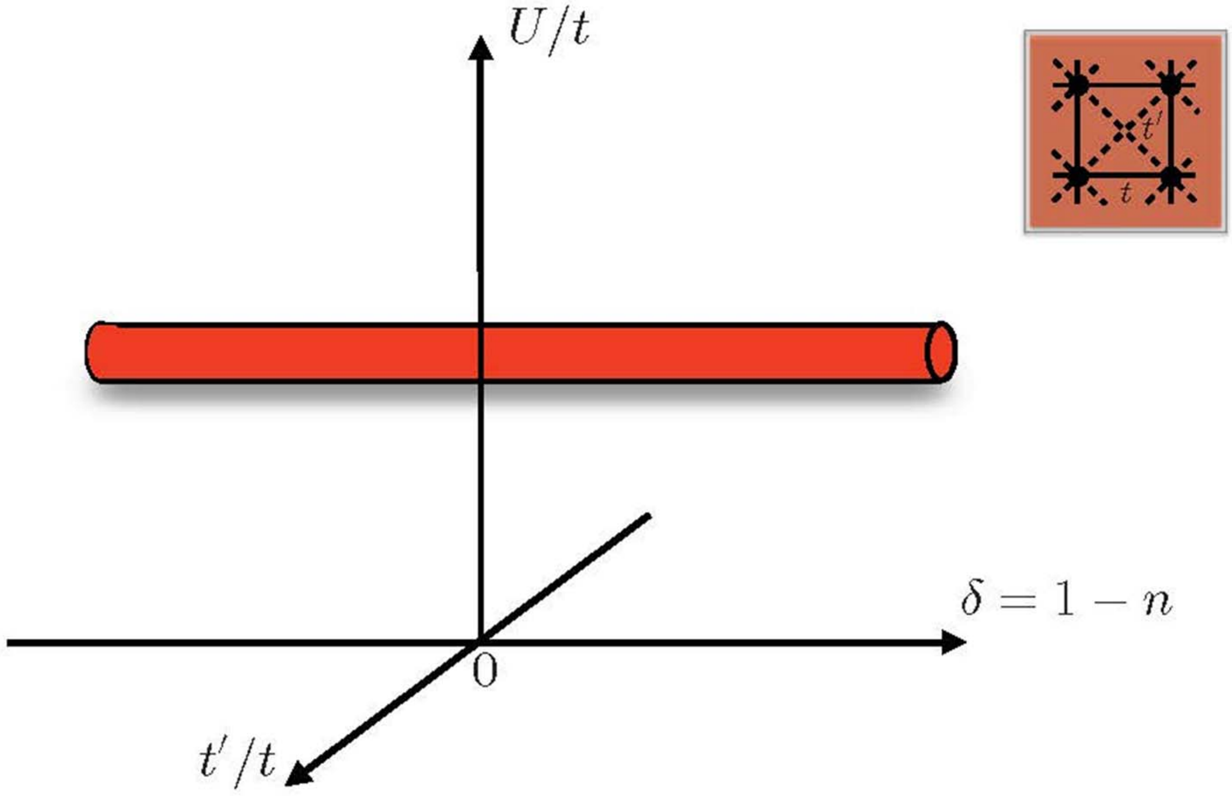


Perspective

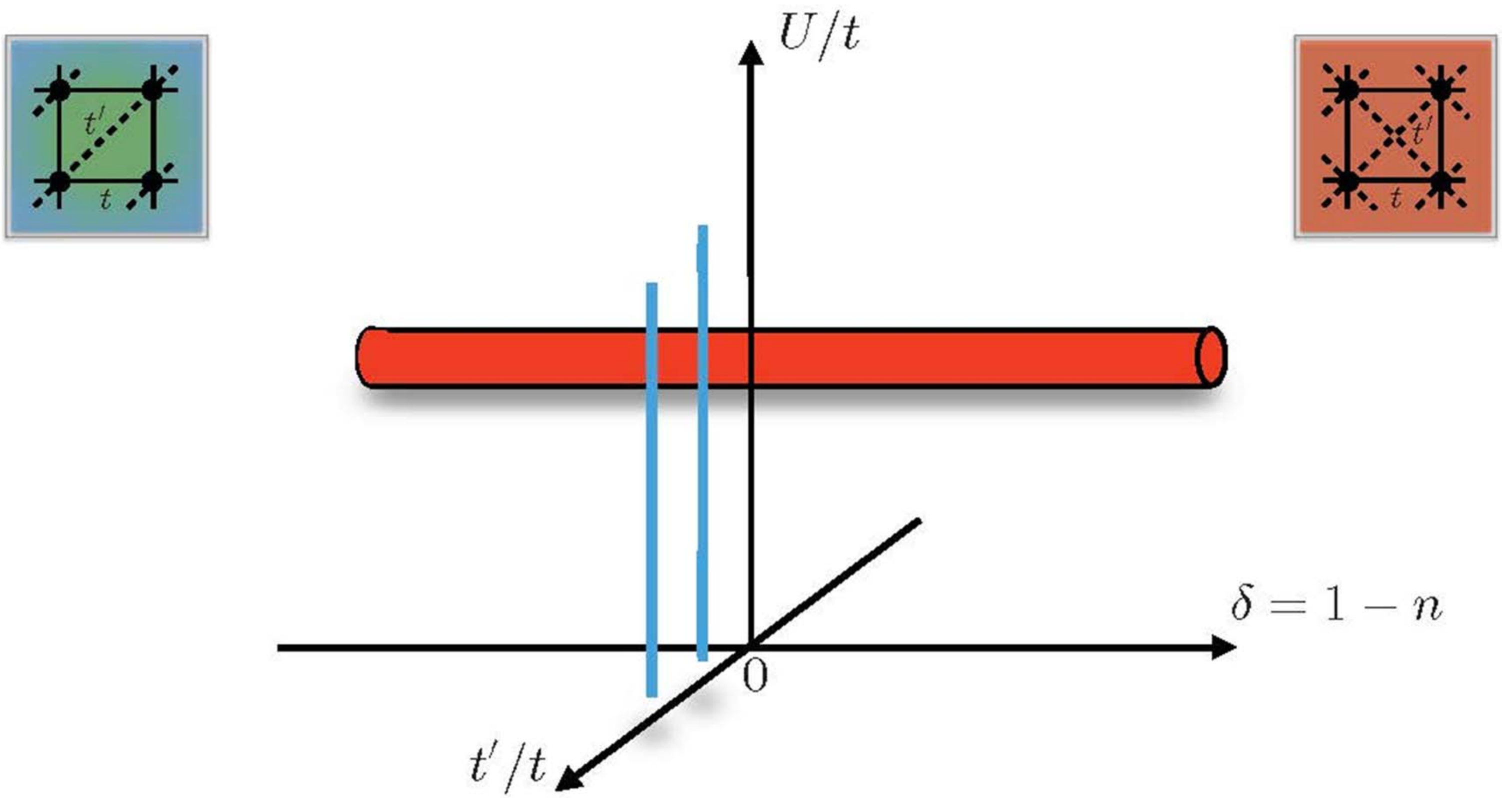




Perspective



Perspective



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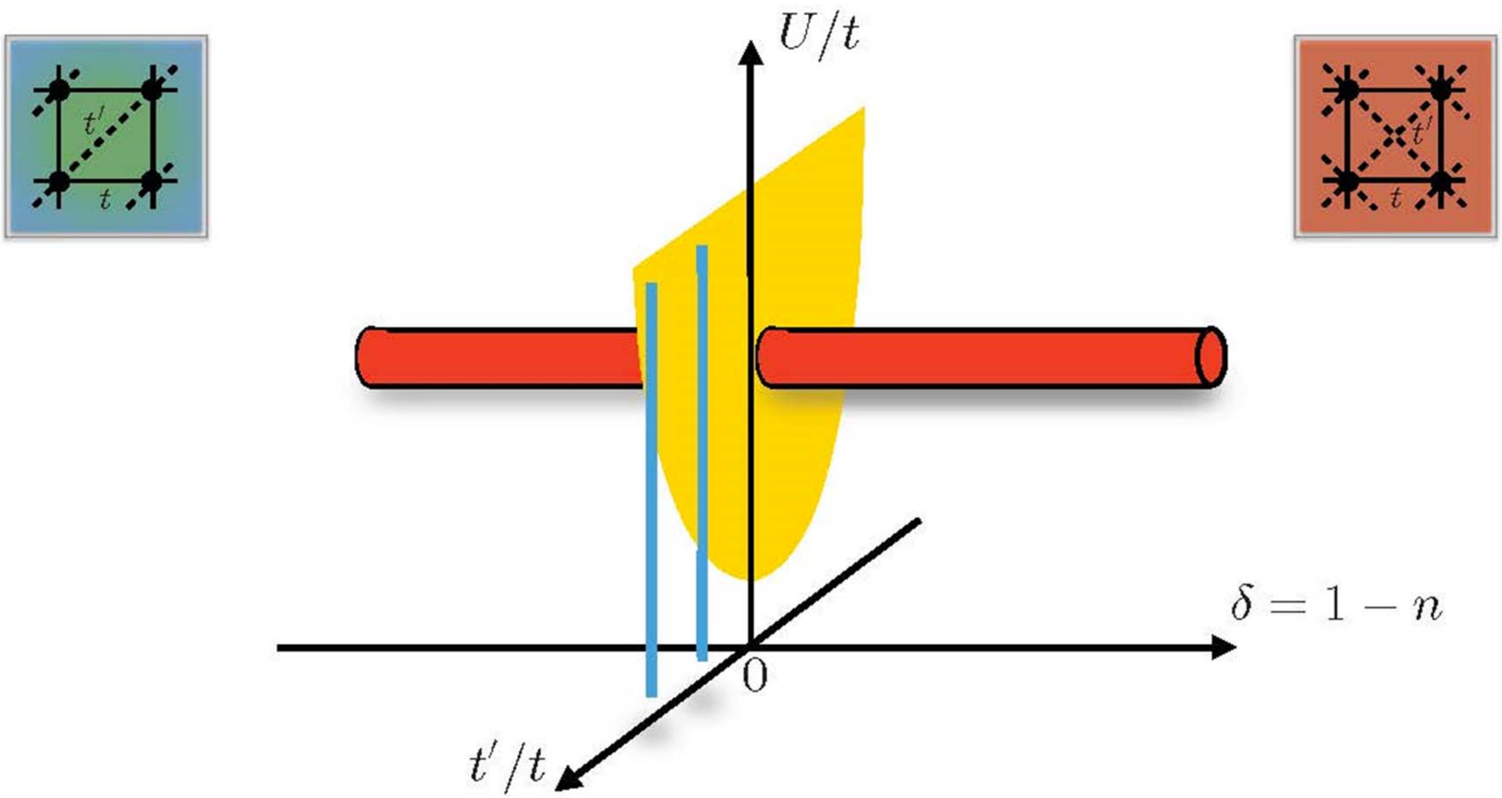
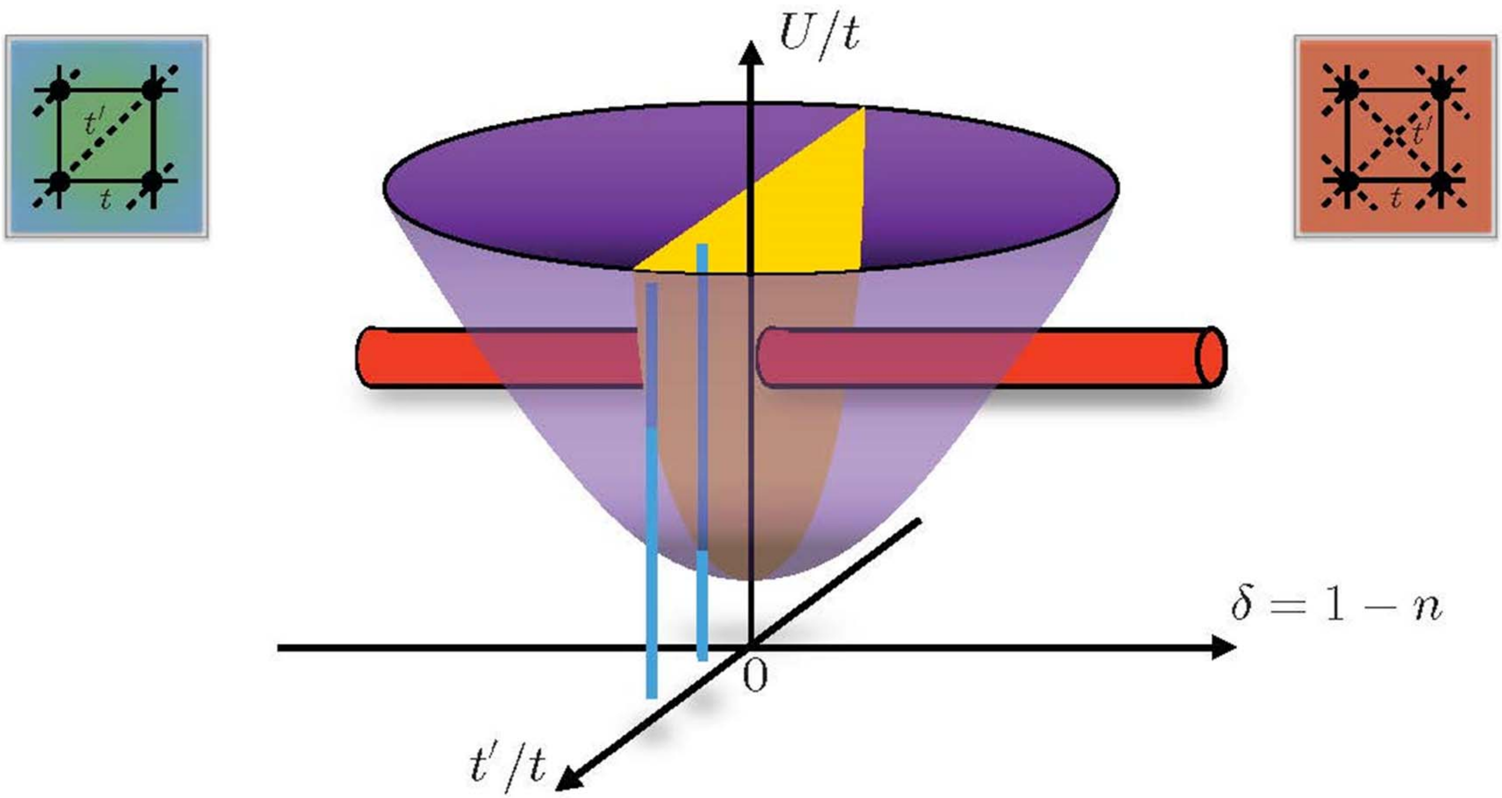
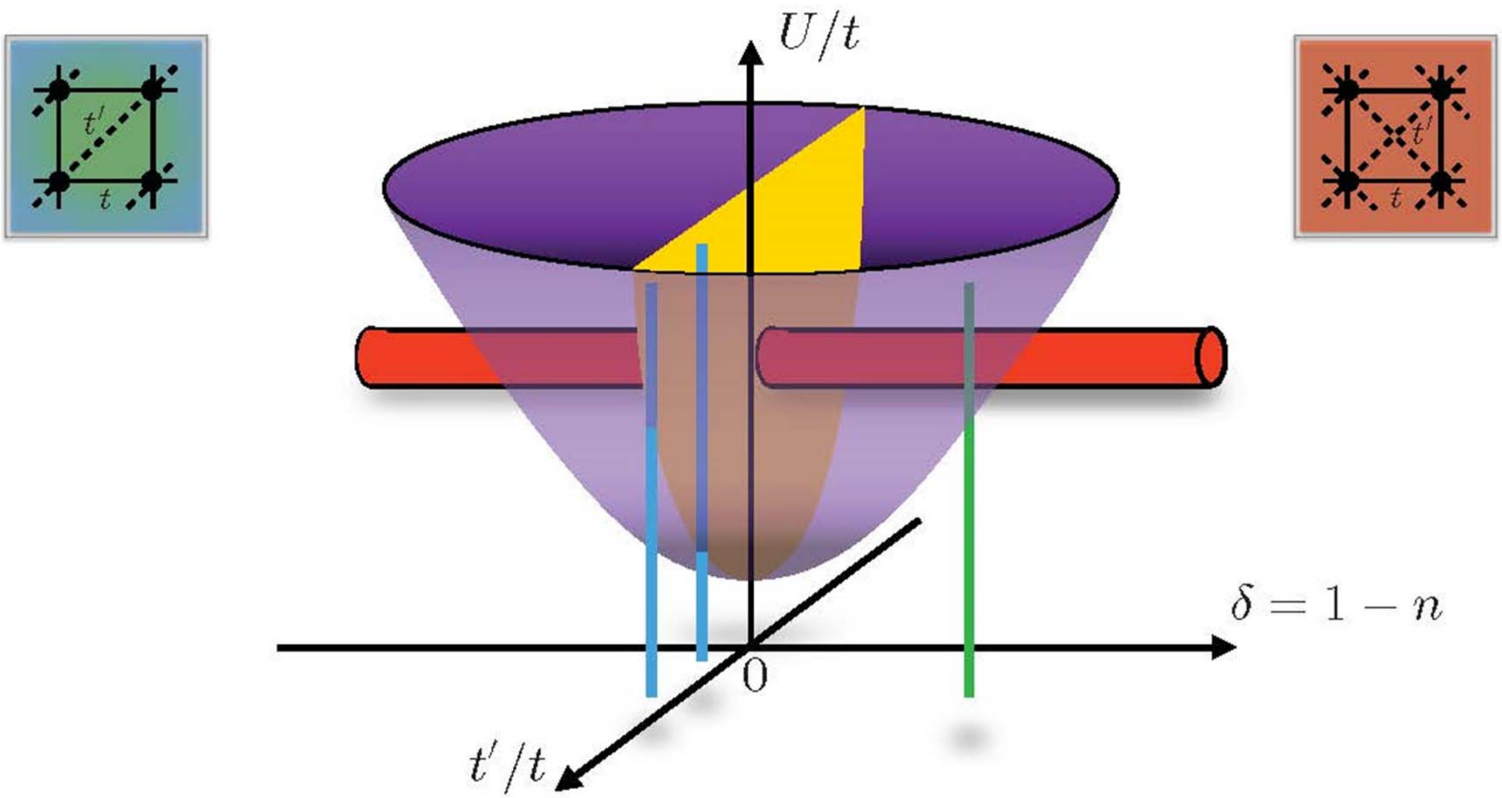
Perspective



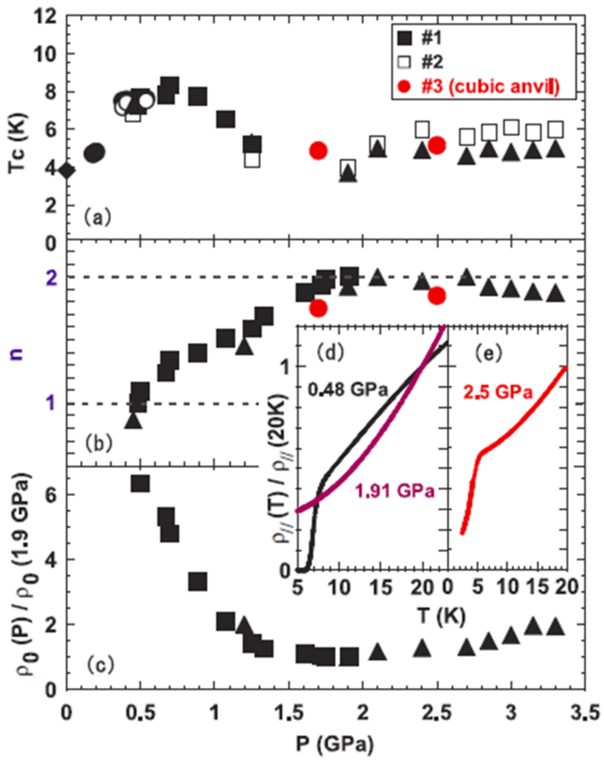
Perspective



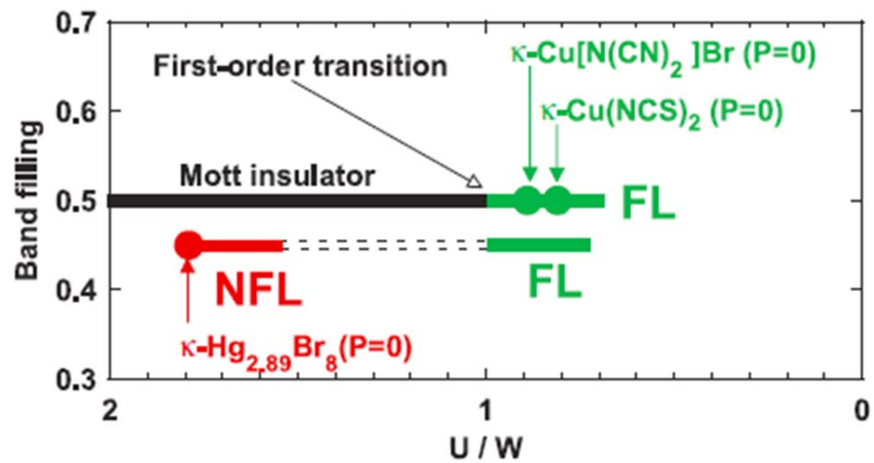
Perspective



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



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

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

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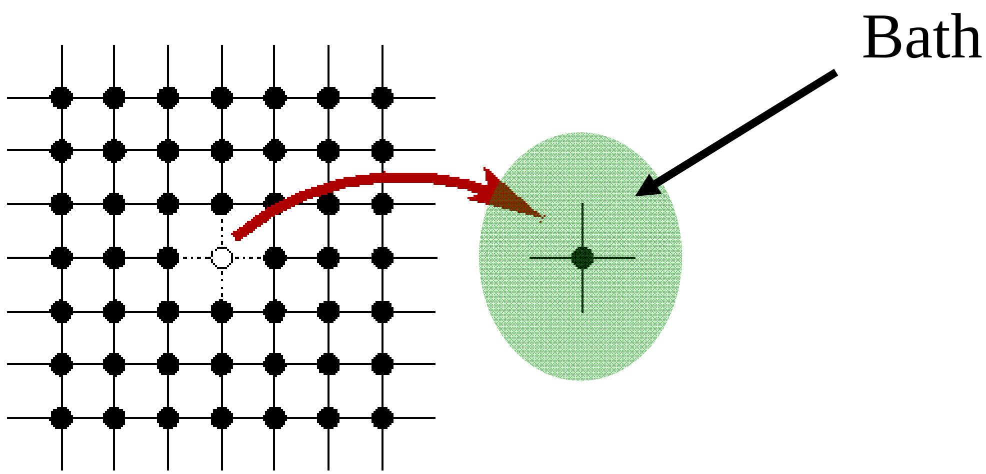
Outline

- Method
- Weak vs strong correlations (AFM and SC)
- Phase diagram
  - $n = 1$
  - finite doping
- What controls maximum T_c ? (Quantum critical point?)

Method

Concept

Mott transition and Dynamical Mean-Field Theory. The beginnings in *d = infinity*



W. Metzner and D. Vollhardt, PRL (1989)

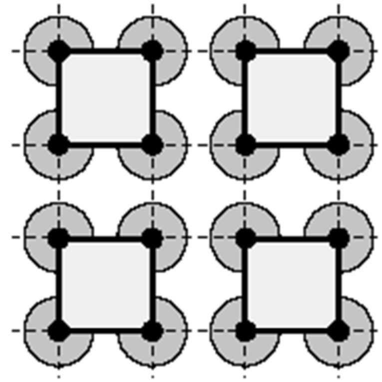
A. Georges and G. Kotliar, PRB (1992)

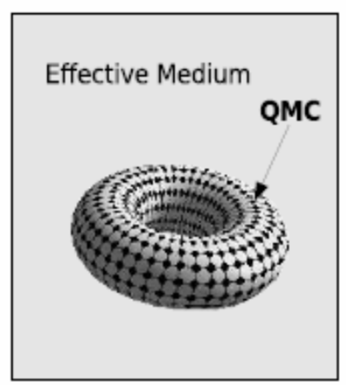
M. Jarrell PRB (1992)

DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method

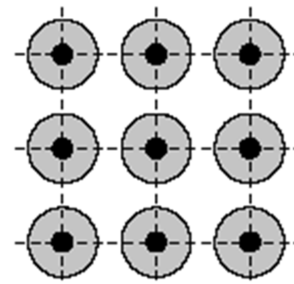
C-DMFT





DCA

DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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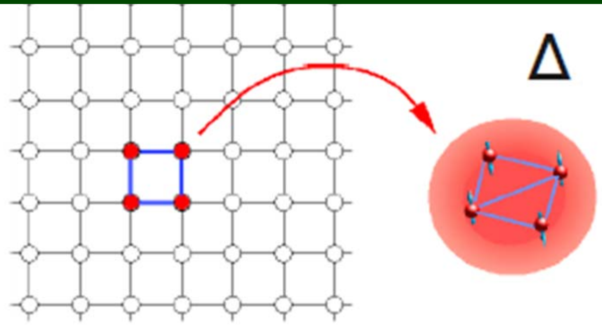
+ and -

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

Method

Tools: Impurity solver

CTQMC impurity solver (tool) (T finite)

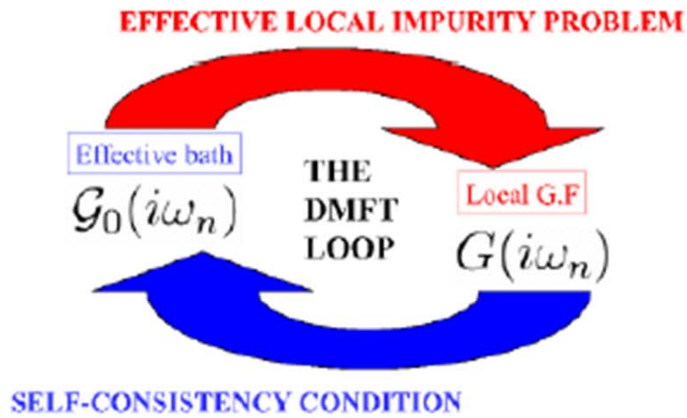


$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau) \Delta_{\mathbf{K}}(\tau,\tau') \psi_{\mathbf{K}}(\tau')}$$

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



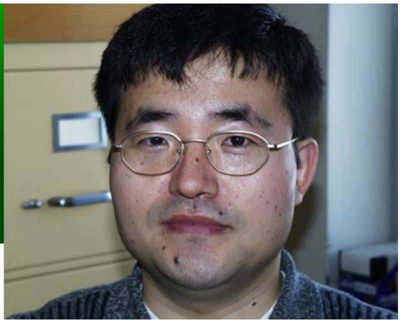
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

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

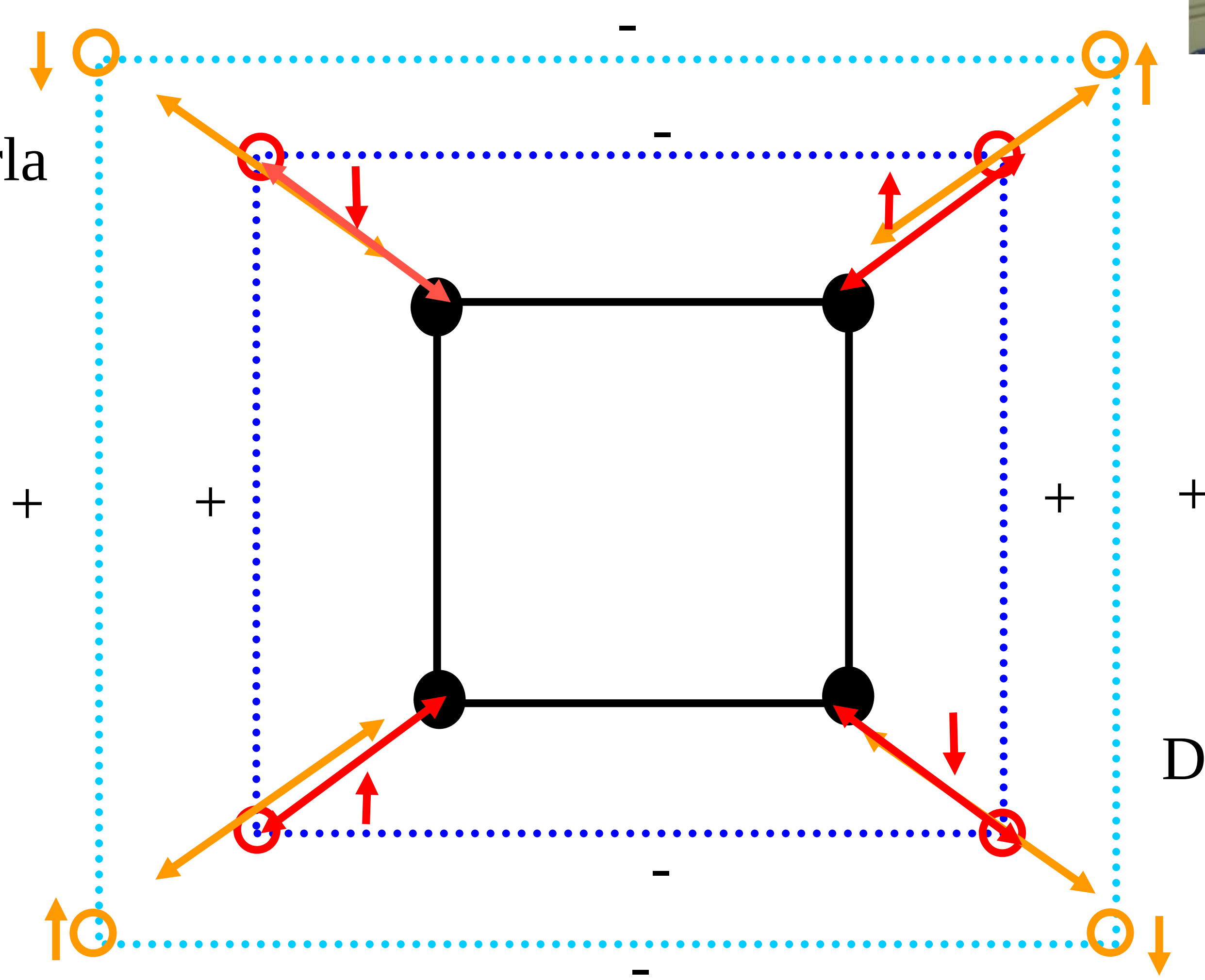
Exact diagonalization impurity solver

ED impurity solver ($T = 0$)

S. Kancharla



B. Kyung



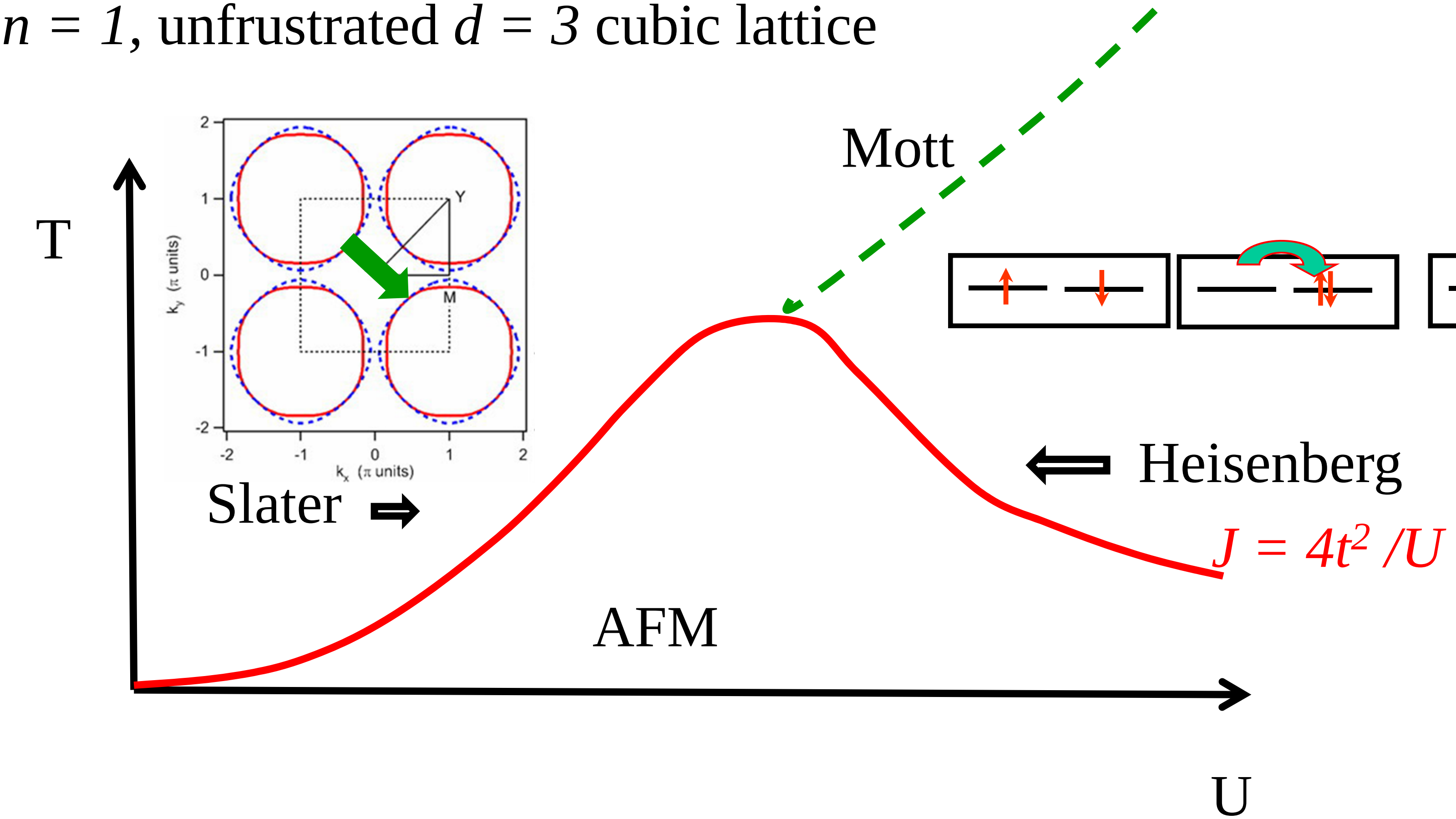
David Sénéchal

Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

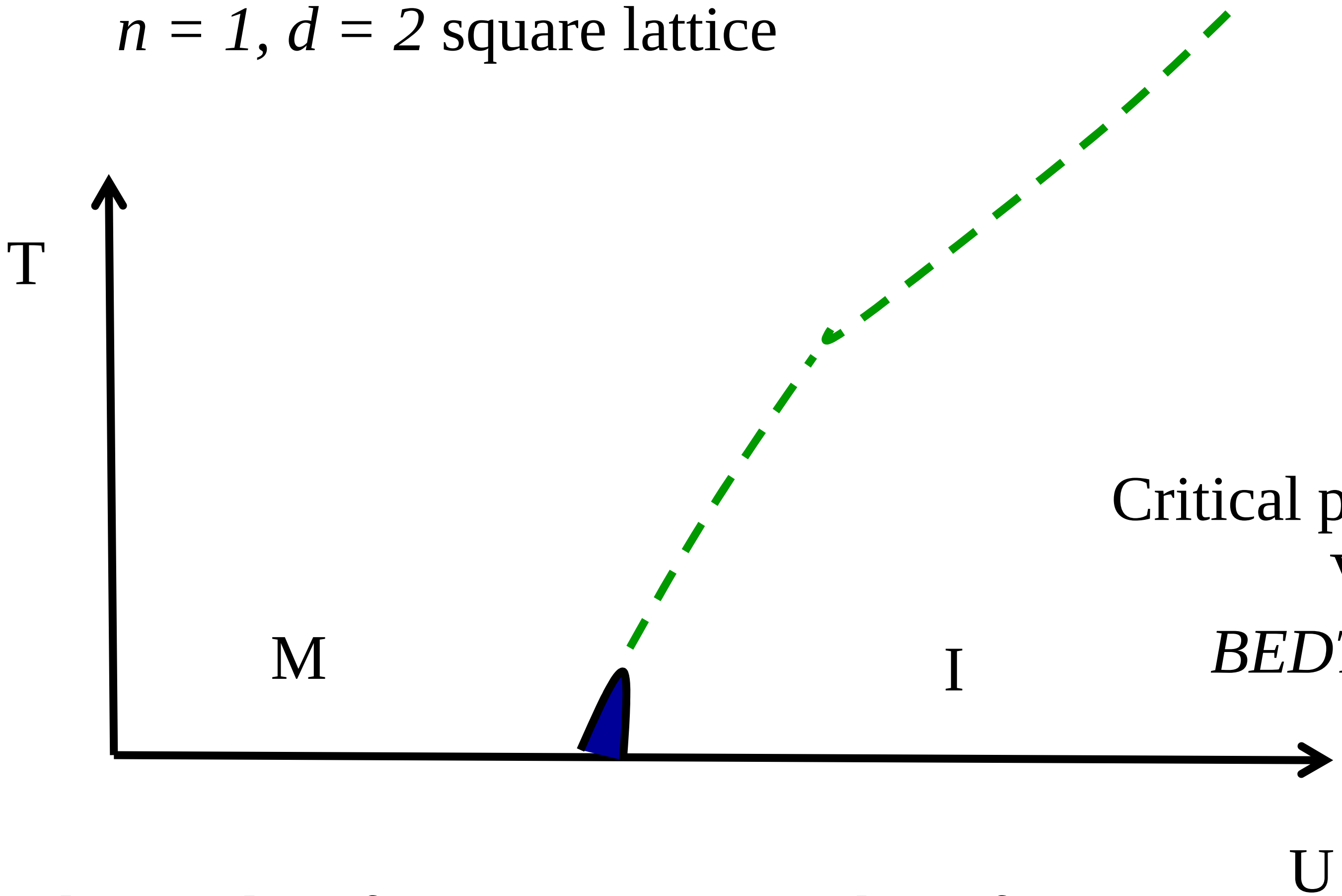
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice



Critical point visible in V_2O_3, *BEDT* organics

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

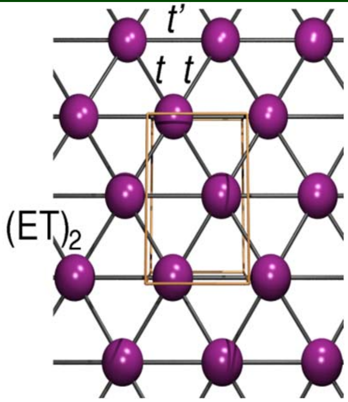
T = 0 phase diagram *n = 1*

Phase diagram

Exact diagonalization as impurity solver ($T=0$).

Other compounds (R. Valenti et al.)

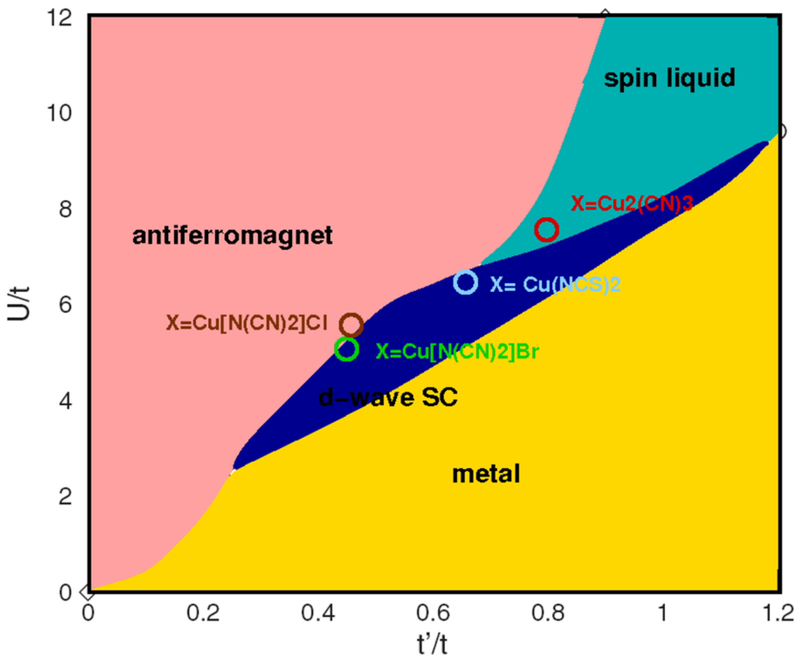
	Hueckel		DFT	
X	t'/t	U/t	t'/t	U/t
CN	1.06	8.2	0.83 (0.85)	7.3 (12)
SCN	0.84	6.8	0.58 (0.83)	6.0
Cl	0.75	7.5	0.44	7.5
Br	0.68	7.2	0.42	5.1



Kandpal et al. PRL (2009)

Nakamura et al. JPSJ (2009)

Komatsu et al. JPSJ (1996)



Kyung, Tremblay PRL (2006)

Tocchio, Parola, Gros, Becca PRB (2009)

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Analogous results with other methods

H. Morita et al., J. Phys. Soc. Jpn. 71, 2109 (2002).

J. Liu et al., Phys. Rev. Lett. 94, 127003 (2005).

S.S. Lee et al., Phys. Rev. Lett. 95, 036403 (2005).

B. Powell et al., Phys. Rev. Lett. 94, 047004 (2005).

J.Y. Gan et al., Phys. Rev. Lett. 94, 067005 (2005).

T. Watanabe et J. Phys. Soc. Japan (2006)

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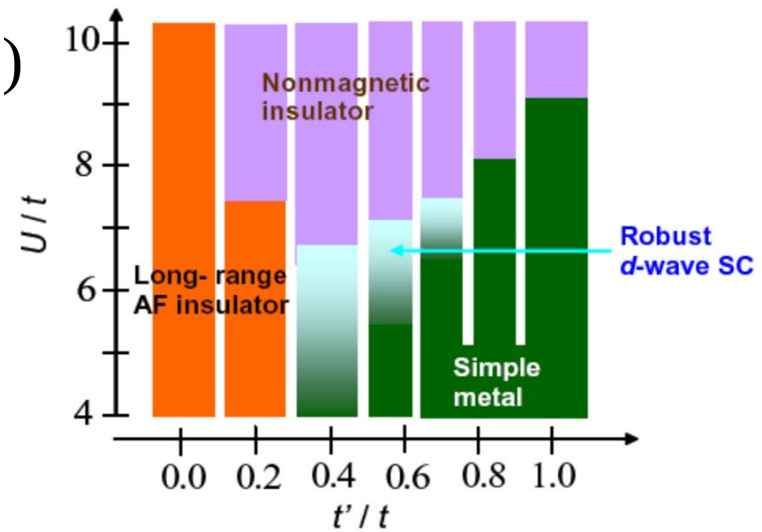

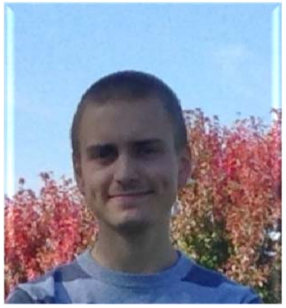

Charles-David Hébert

Patrick Sémon

$n = 1$, normal state, 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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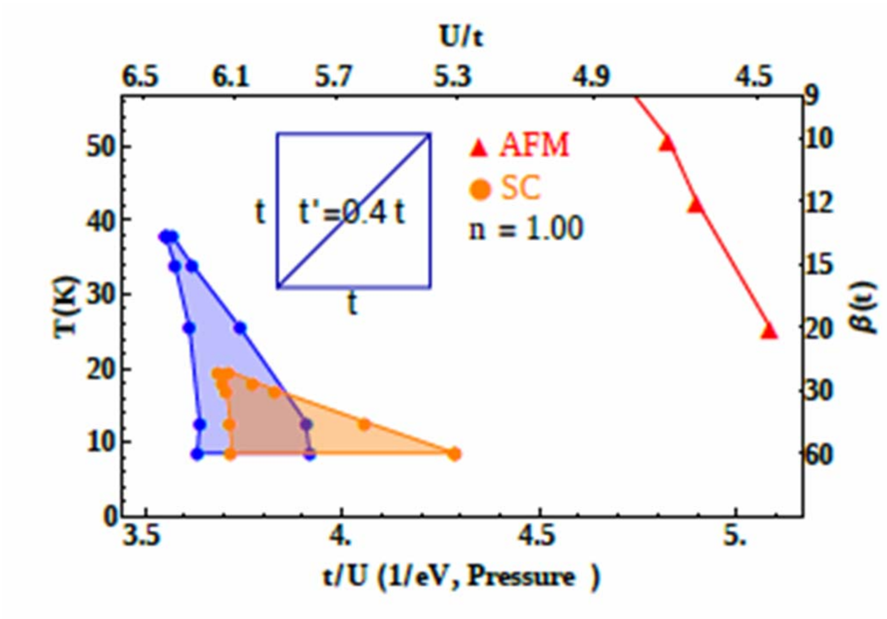
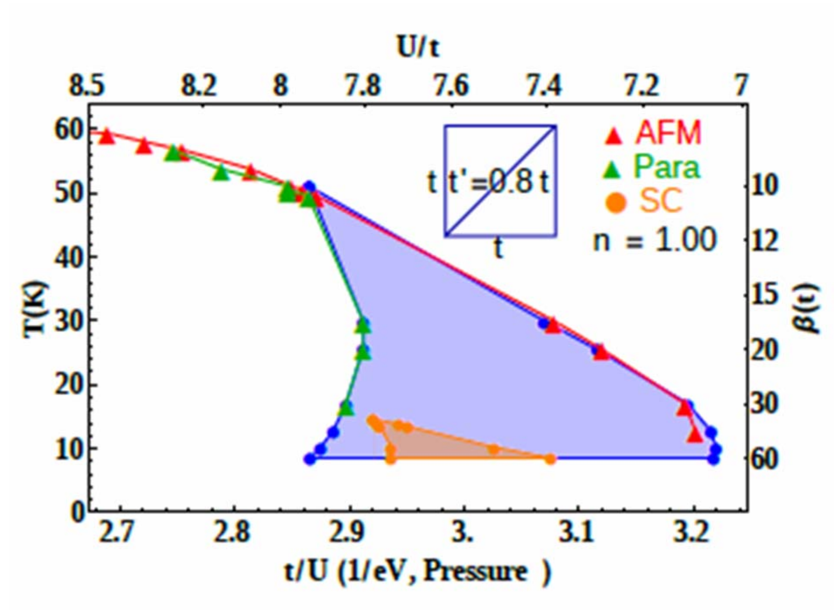
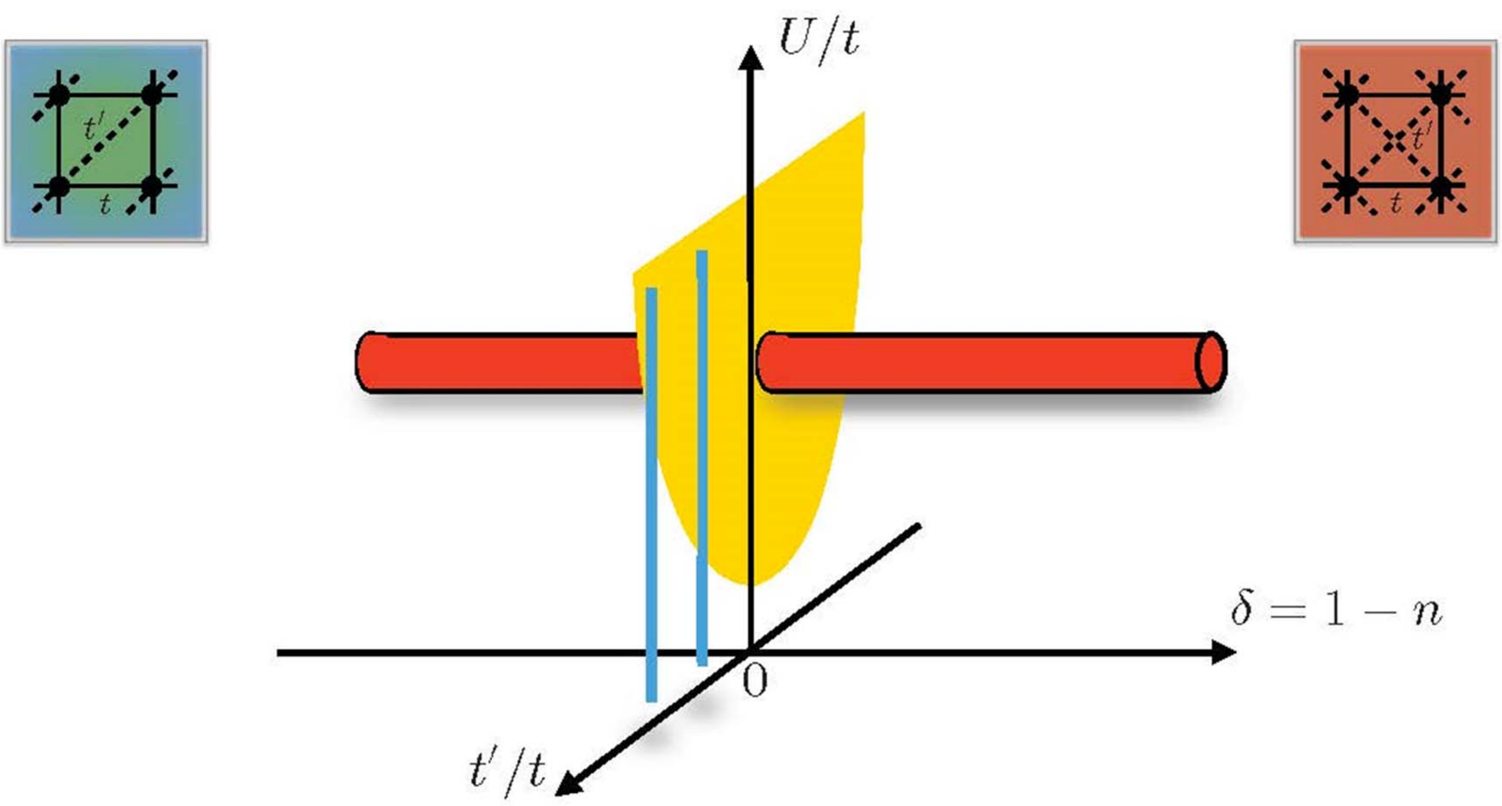
Effect of frustration on Mott transition ($n = 1$)



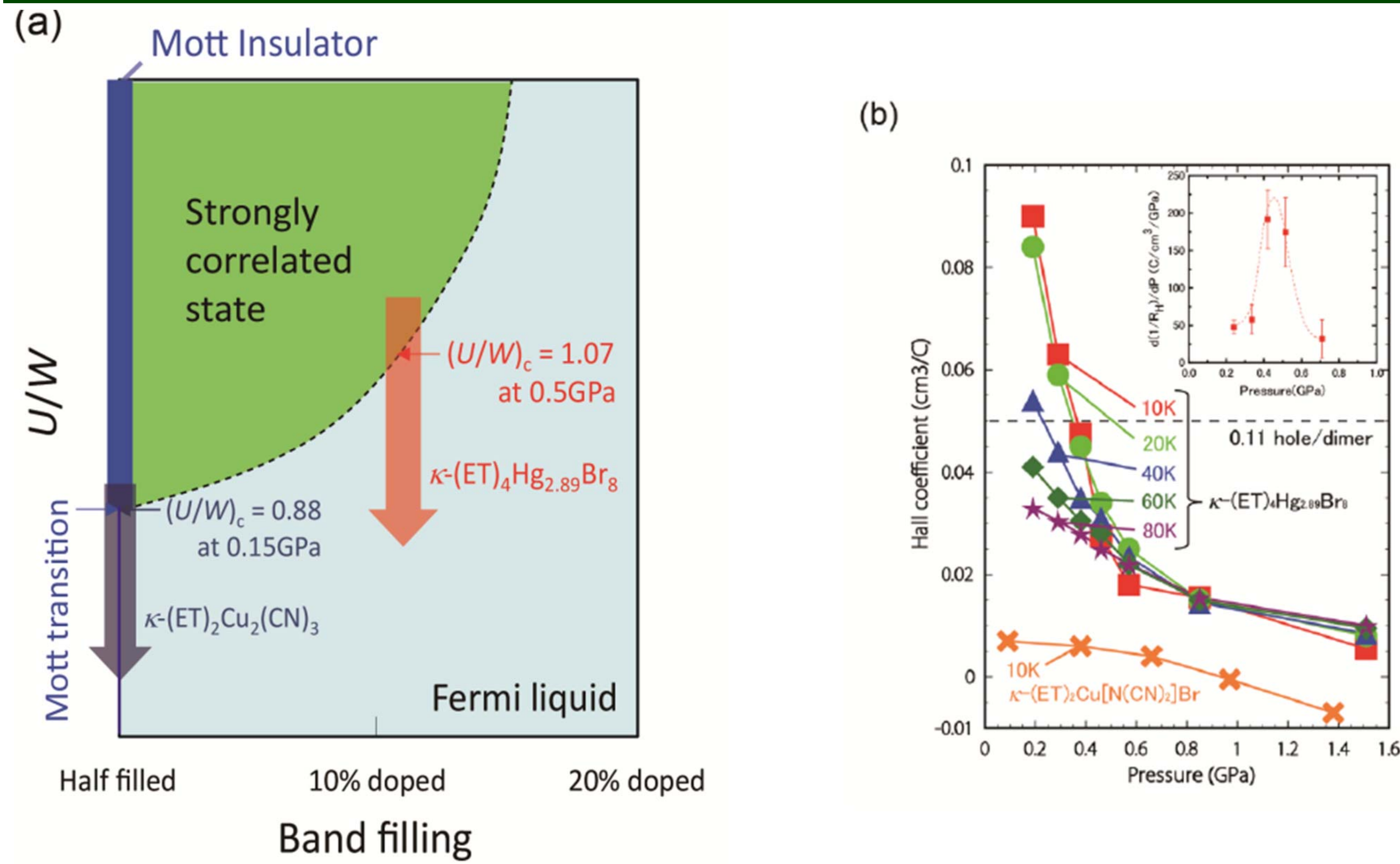


Perspective



Doped Organics: normal state

Doped BEDT



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

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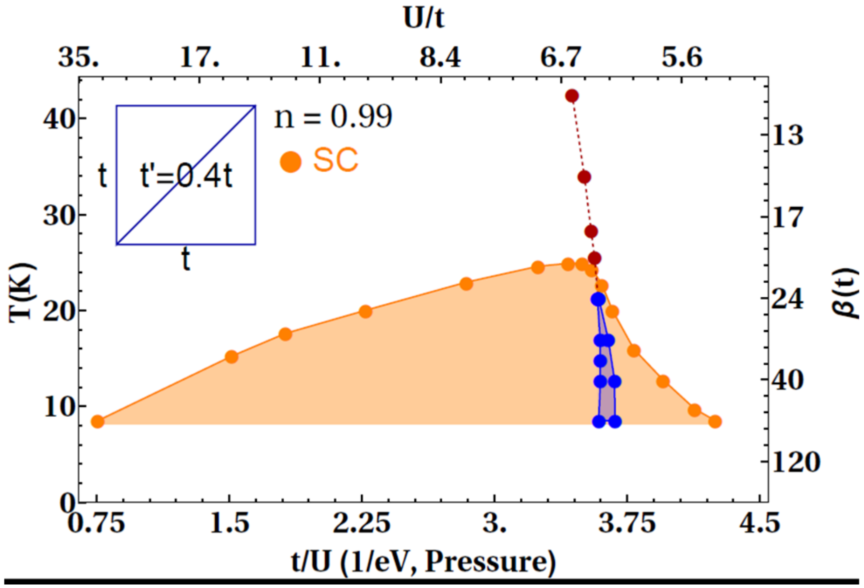
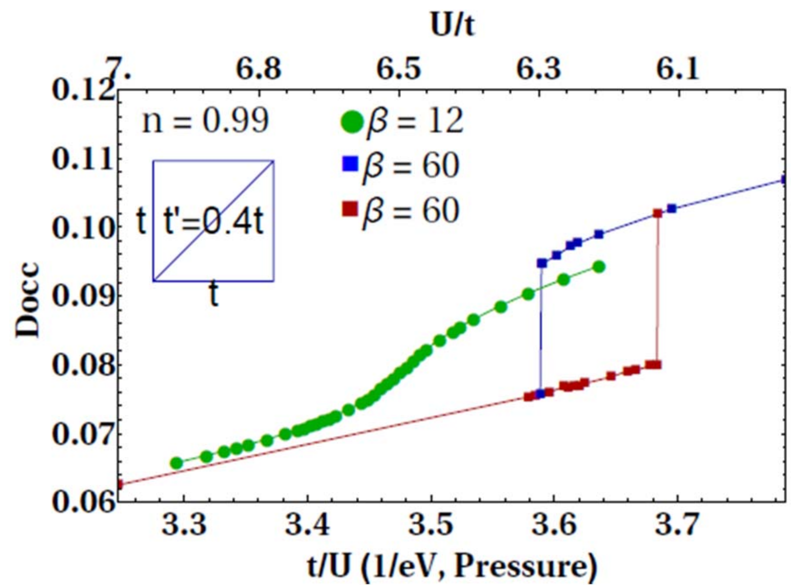
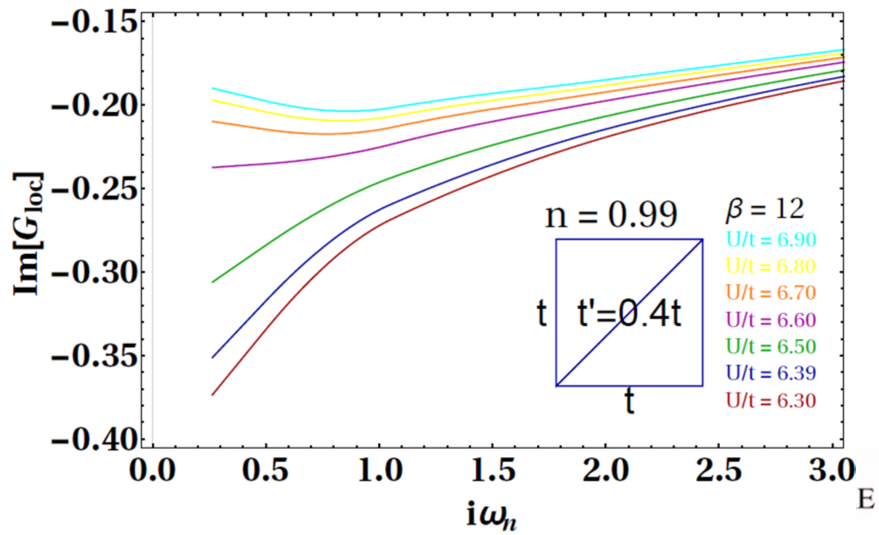
First order and Widom line in organics

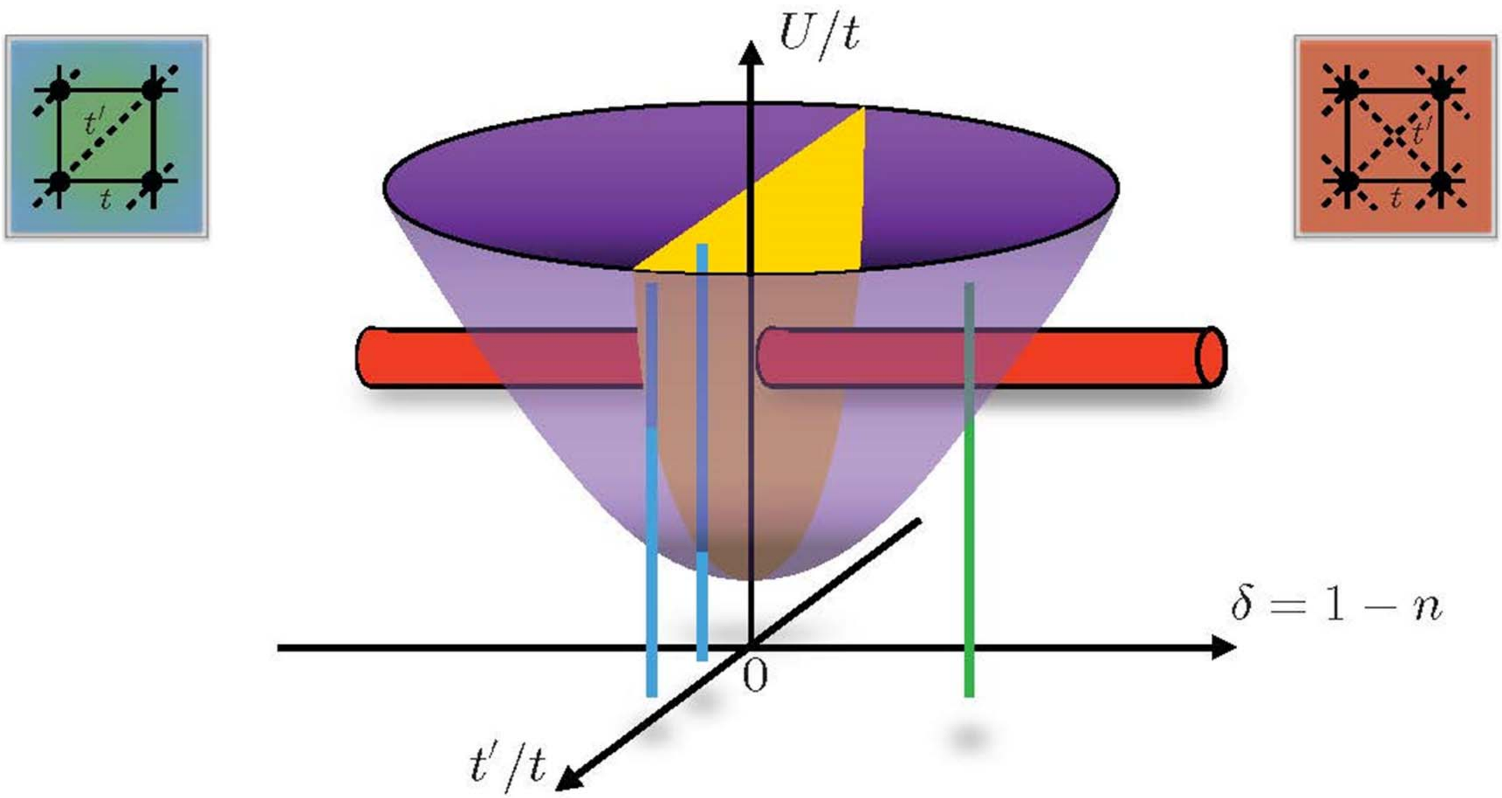




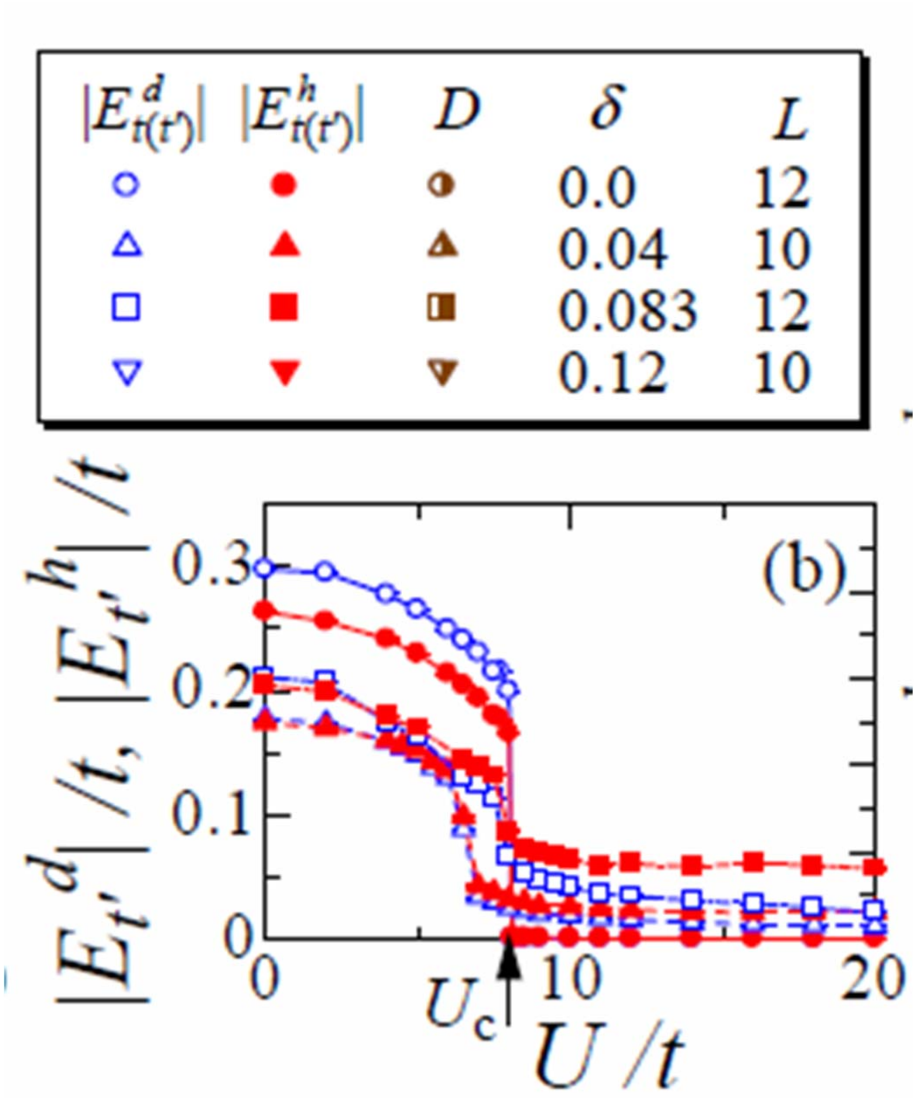


Charles-David Hébert, Patrick Sémon , AMT

Perspective



Results from variational MC



t'/t = 0.8

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

Superconductivity in the organics at finite T

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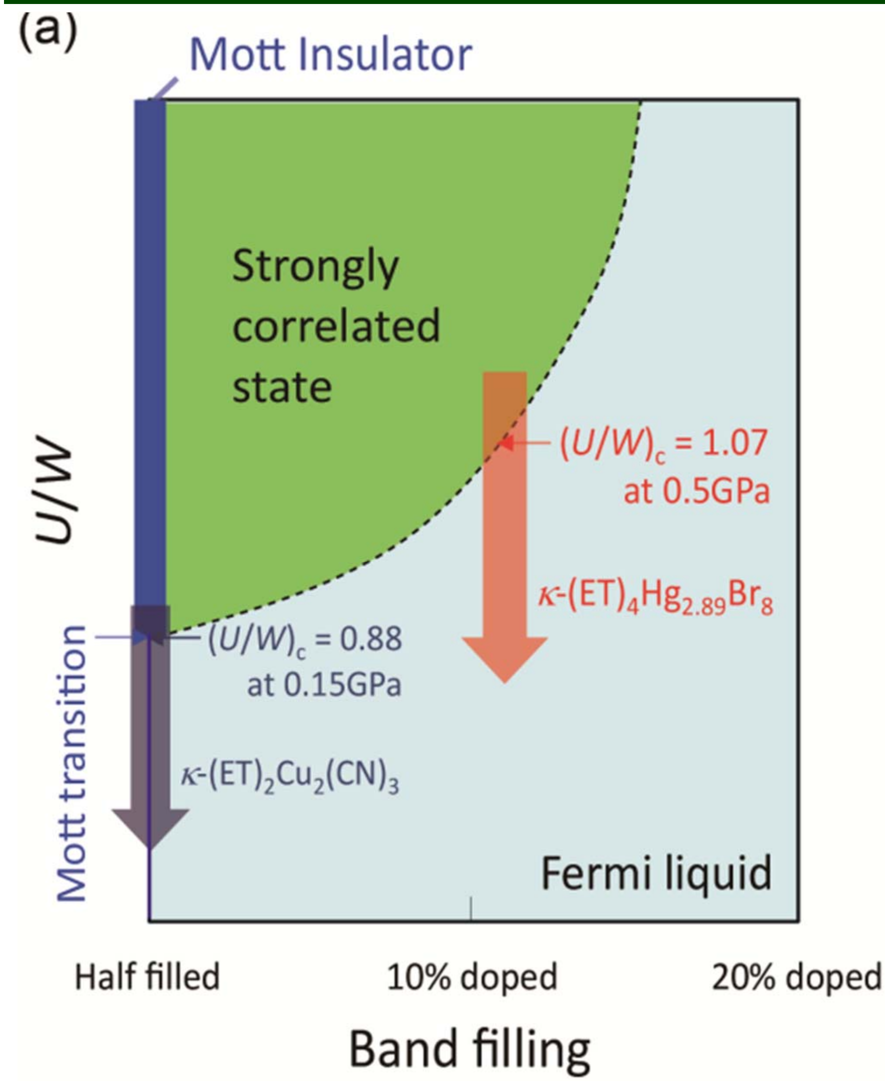
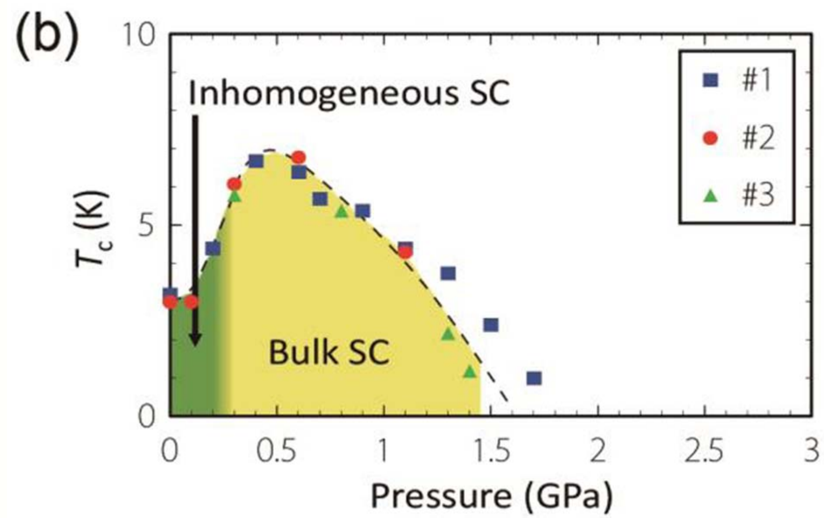
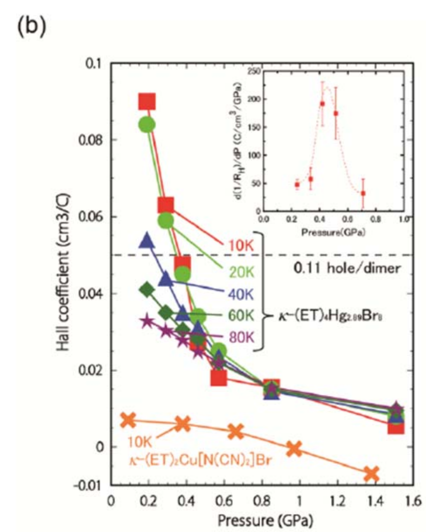
Doped BEDT

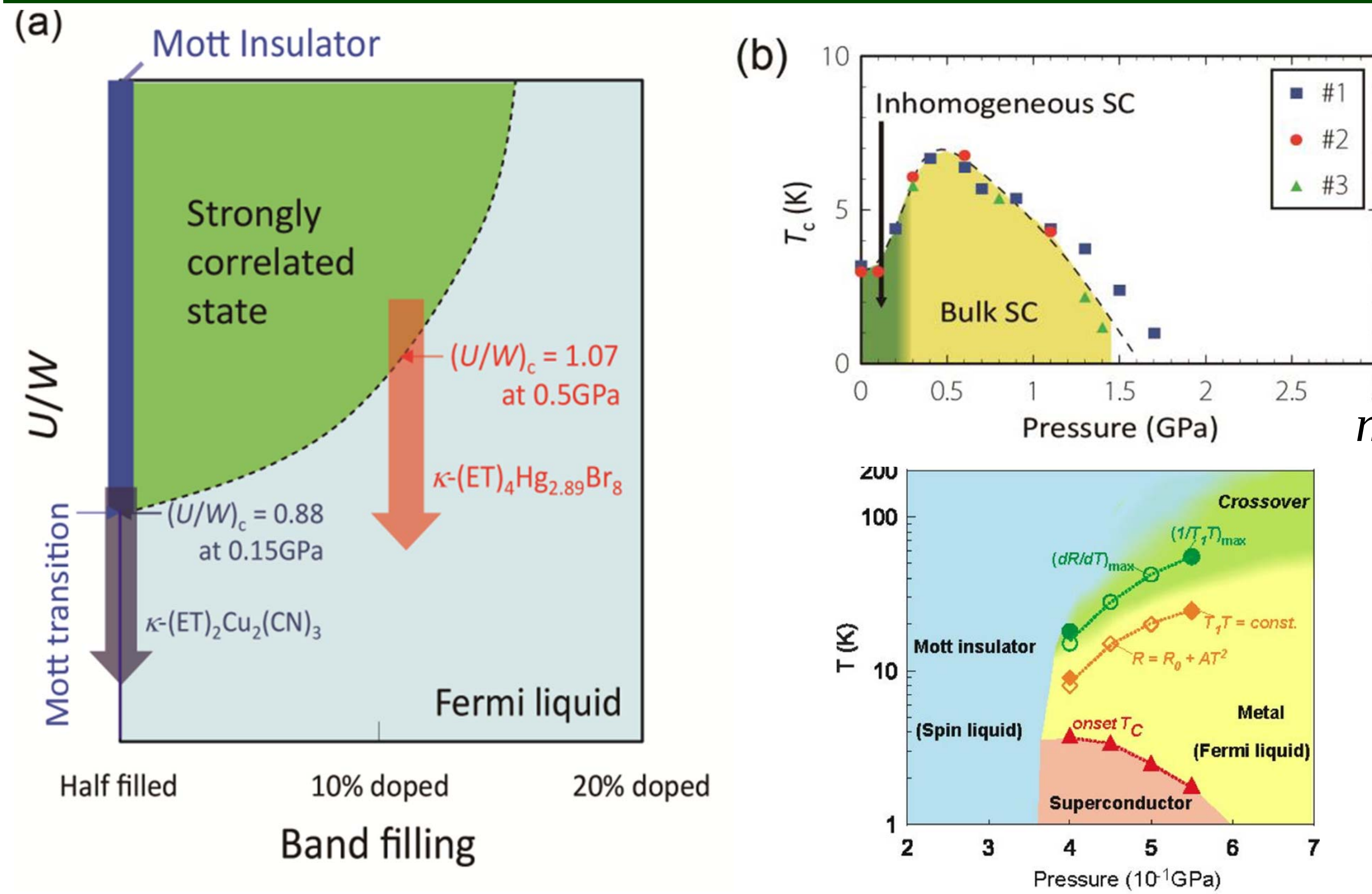






H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Doped BEDT



$n = 0.90$

$n = 1$

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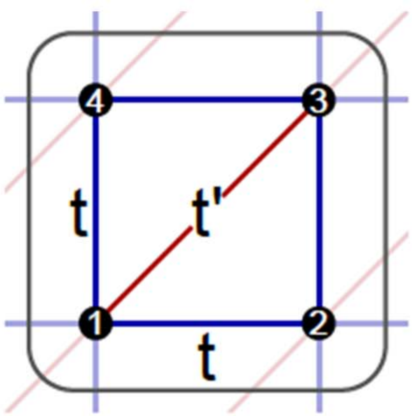
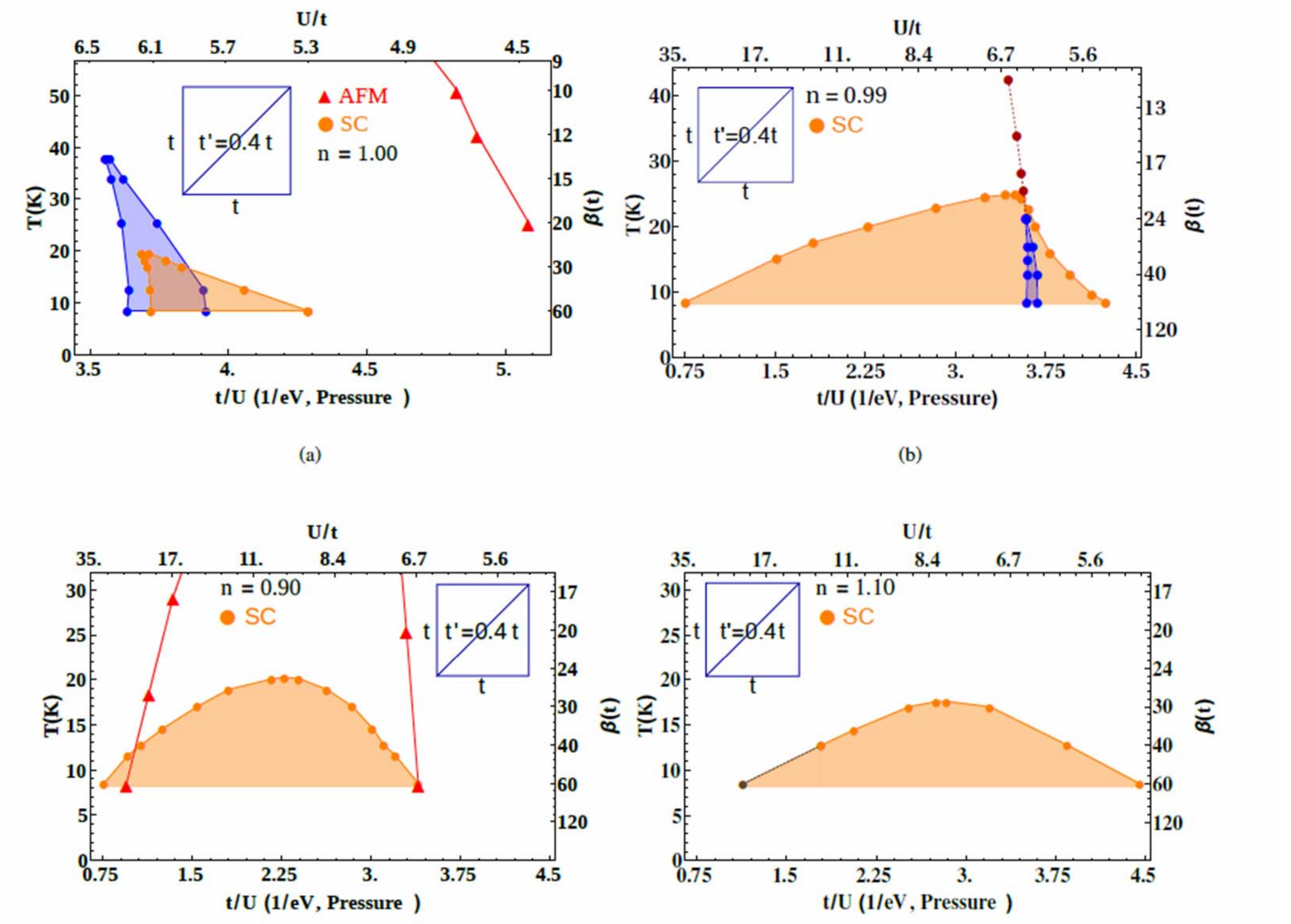
t'=0.4t





(a) (b) (c) (d)

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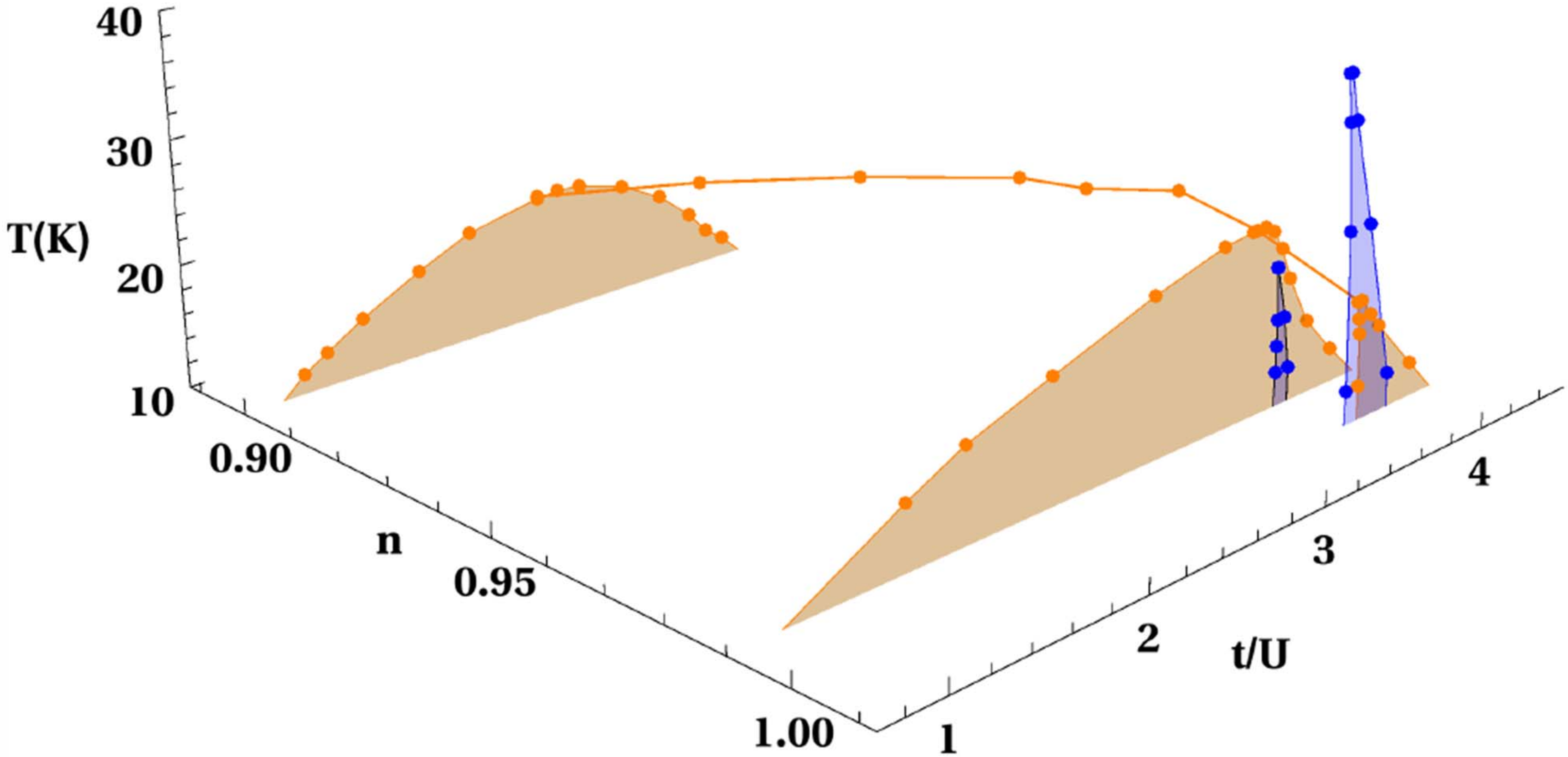
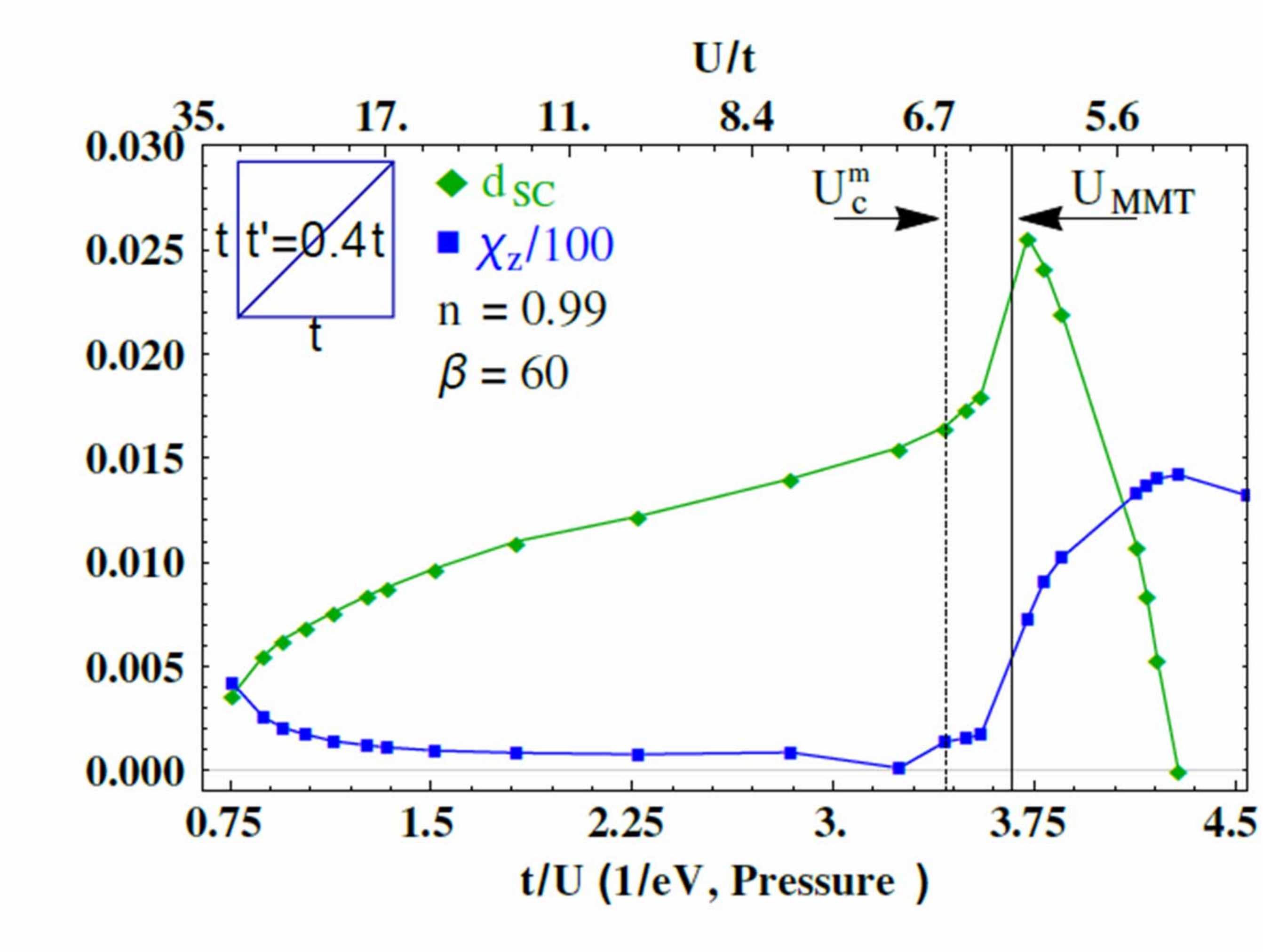
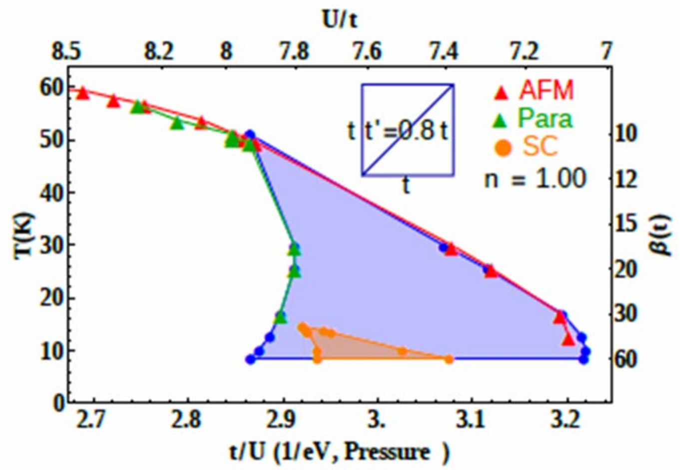
$t' = 0.4t$ overview



Signatures of Widom line in the superconducting state

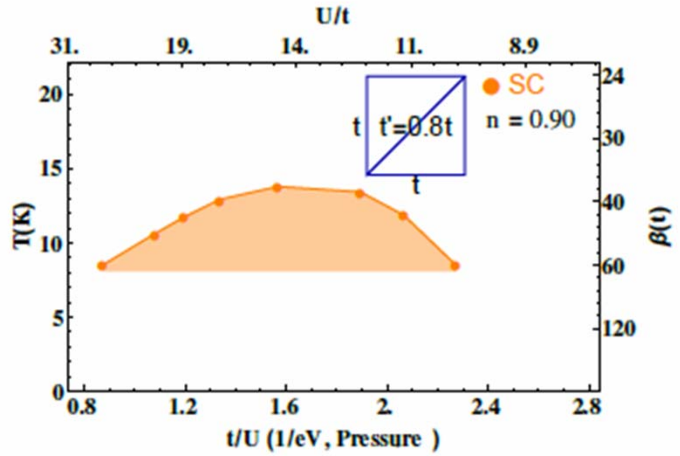


t' = 0.8 t



U/t
8.5
8.2
8
7.8
7.6
7.4
7.2
7
AFM
Para
SC
n = 1.00
t
t'=0.8 t
t
T(K)
β(t)
t/U (1/eV, Pressure)

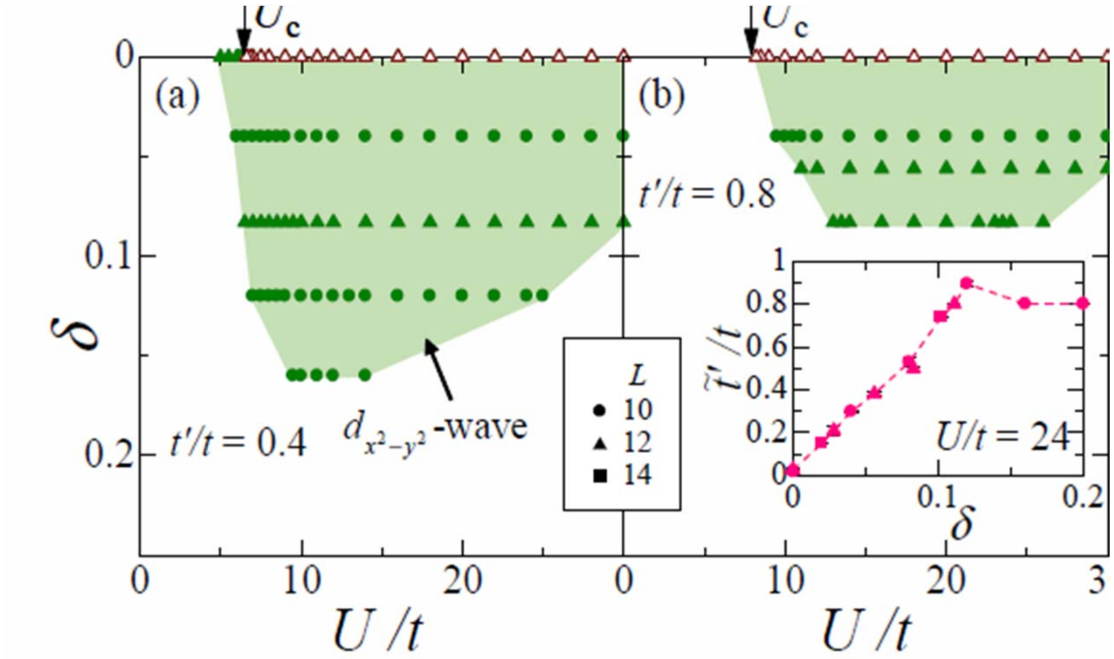
(a)



U/t
31.
19.
14.
11.
8.9
SC
n = 0.90
t
t'=0.8t
t
T(K)
β(t)
t/U (1/eV, Pressure)

(b)

Results from variational MC

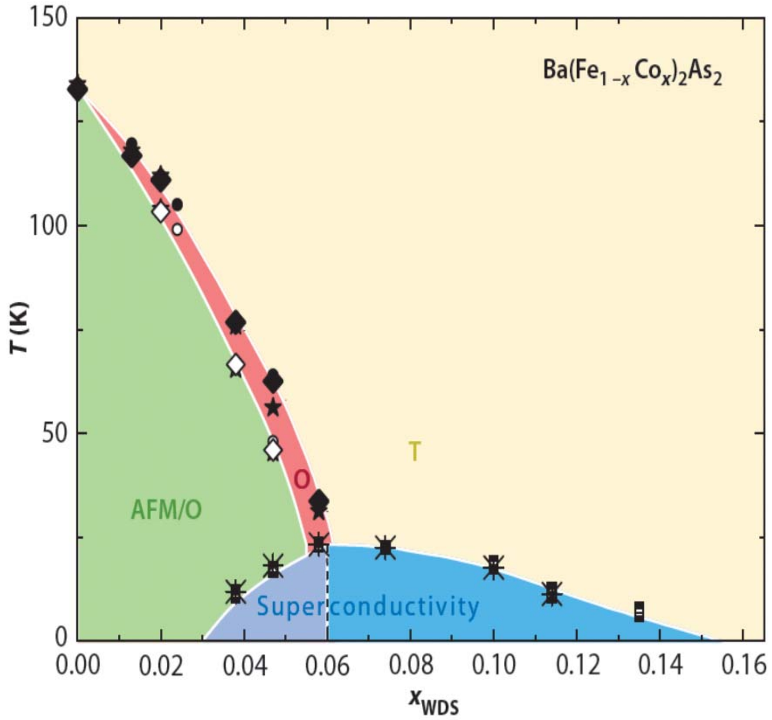


T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

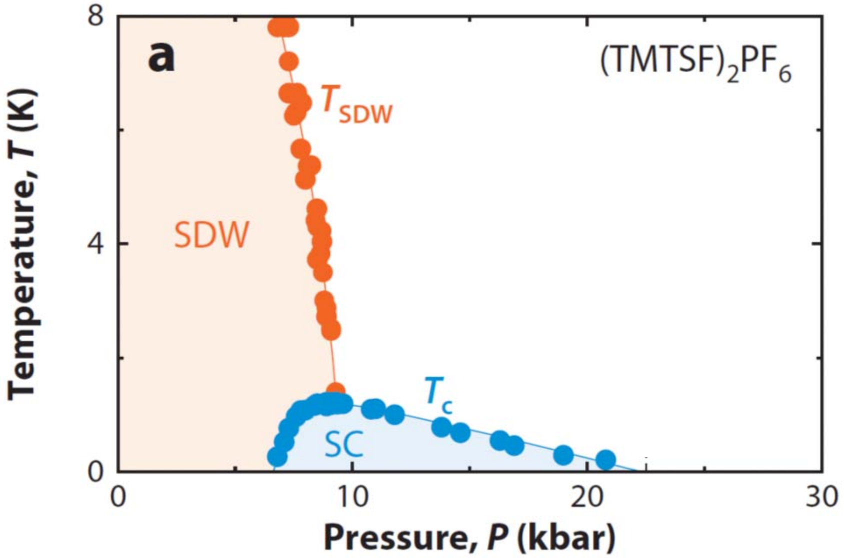
Antiferromagnetic quantum critical point scenario (weakly correlated)

Pnictides and organics

Pnictides



Organics



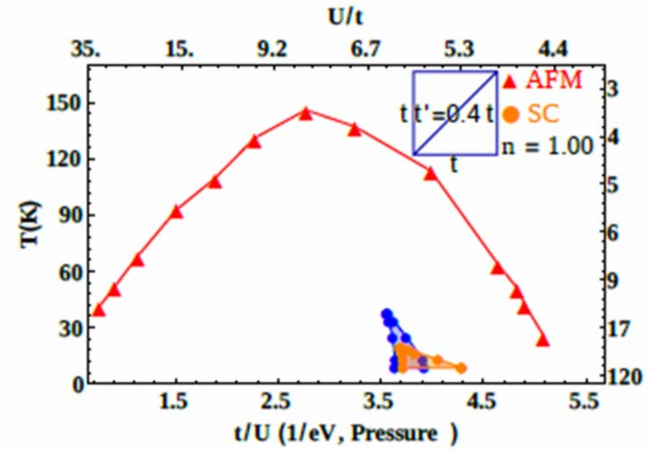
The Archetype

Magnetic superconductivity

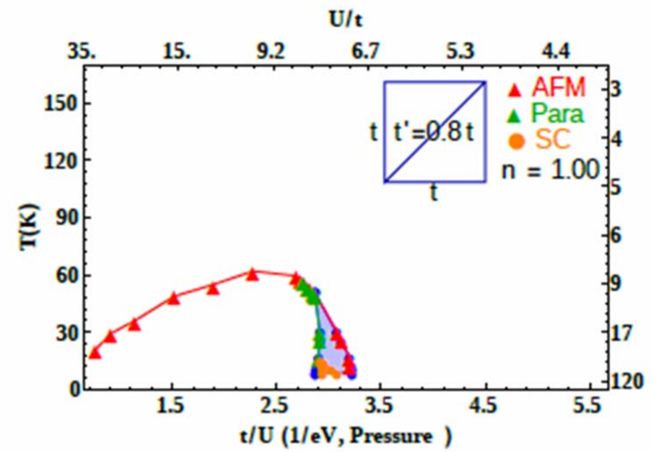
Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

Canfield et al. (2010)

AFM not related to maximum T_c



(a)



(b)

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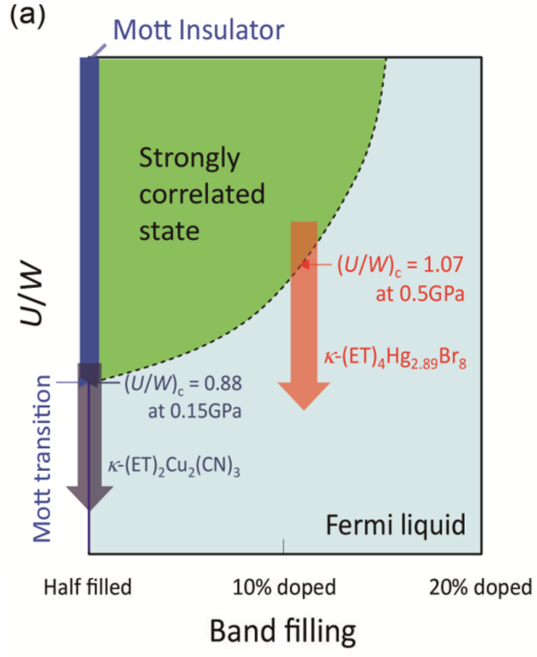
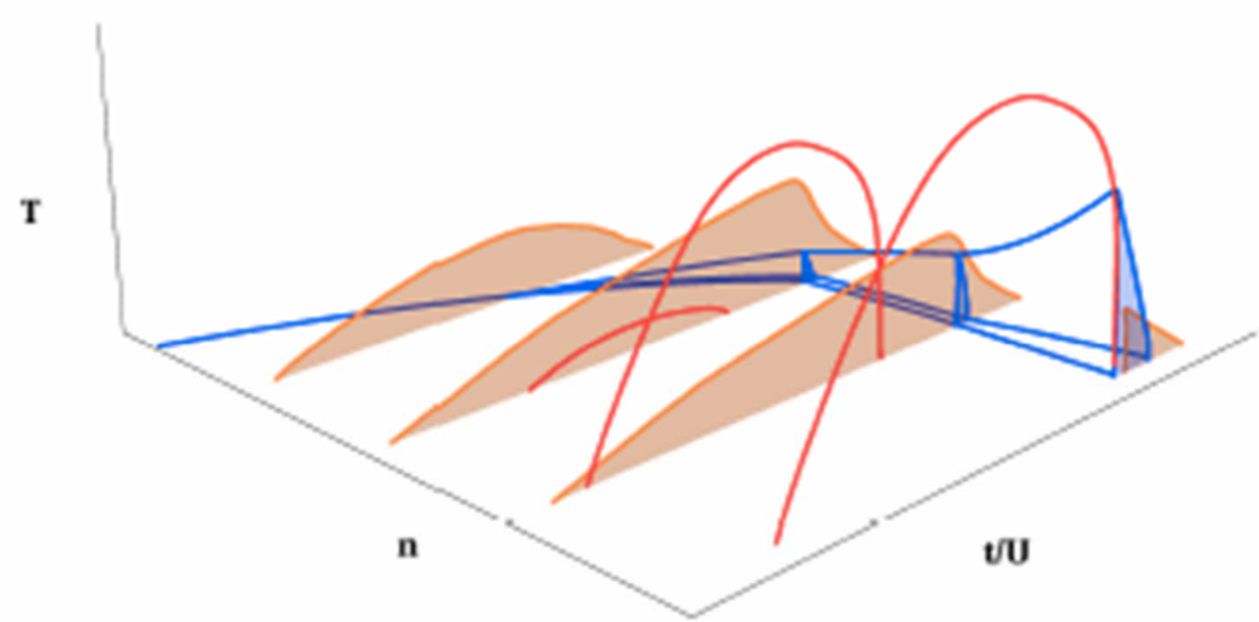
Generic case highly frustrated case





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

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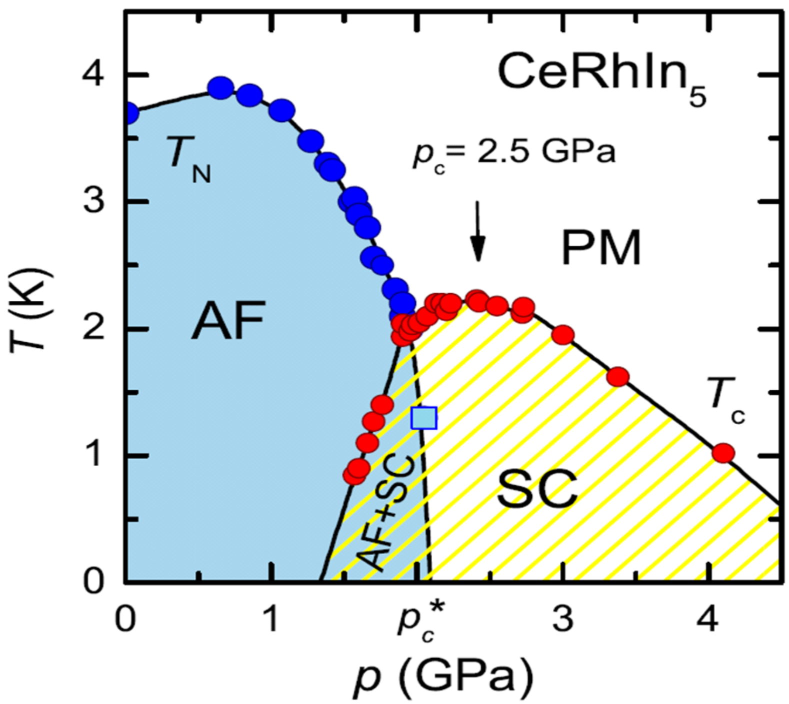
Heavy fermions

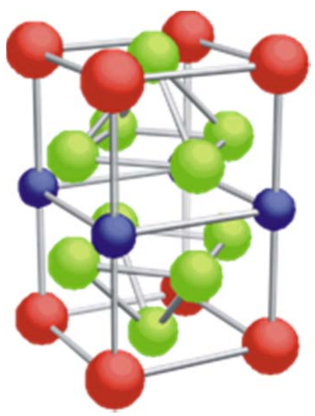
Heavy fermions **3D metals tuned by pressure, field or concentration**



Knebel et al. (2009)

Quantum criticality

$CeRhIn_5$



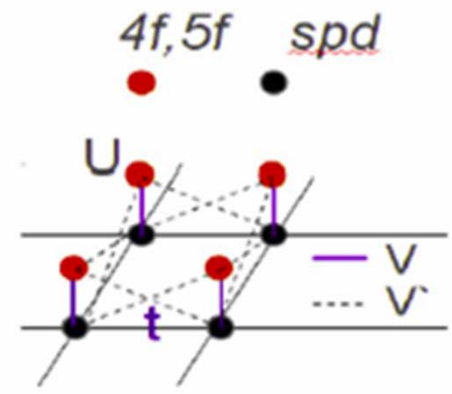
Magnetic superconductivity

Mathur et al., Nature 1998

Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$

$$+ \sum_{k,\sigma} V_k (f^\dagger_{k,\sigma} c_{k,\sigma} + \mathrm{H.c.}) + \sum_i U \left(n_f^\uparrow - \frac{1}{2}\right)\left(n_f^\downarrow - \frac{1}{2}\right)$$

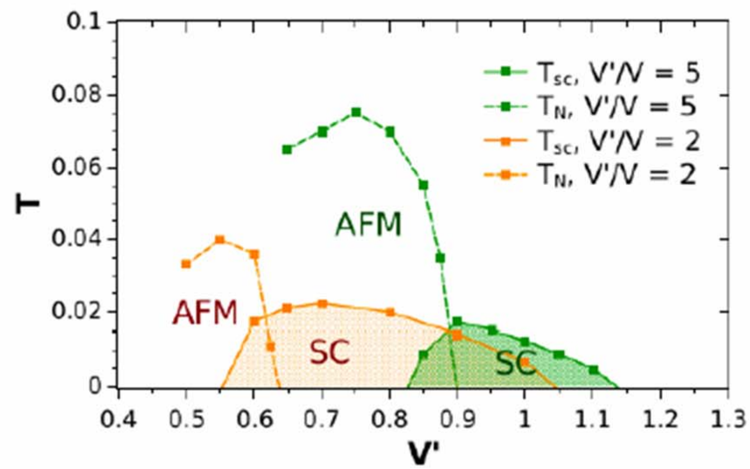


$$V_k = V + 2V'[cos(k_x) + cos(k_y)]$$

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2 : more frustrated case
V'/V = 5 : less frustrated case



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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Main collaborators

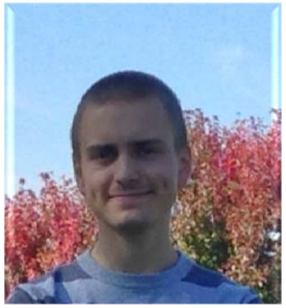
David Sénéchal

Patrick Sémon

Giovanni Sordi

Kristjan Haule

Bumsoo Kyung



Charles-David Hébert

Wei Wu

Lorenzo Fratino

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Team

Tremblay, Reymbaut, Gagnon, Verret, Hébert, Charlebois, Nourafkan

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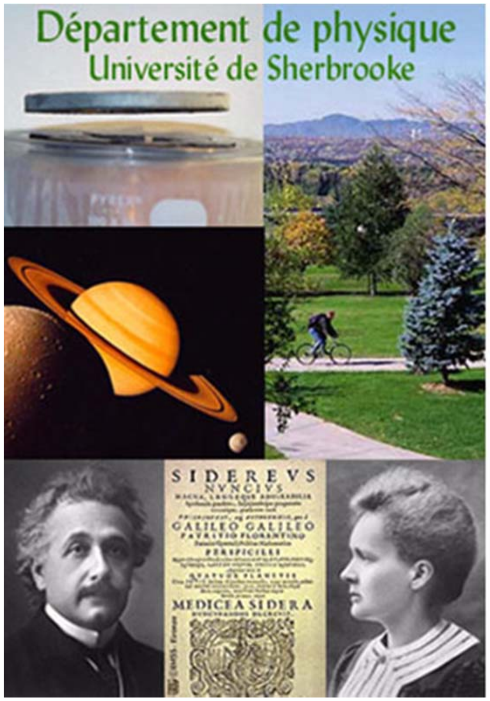

André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP
Le regroupement québécois sur les matériaux de pointe

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

Merci

Thank you

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