Workshop on
Novel Aspects of Superconductivity

Aspen, 31 July 2007

André-Marie Tremblay

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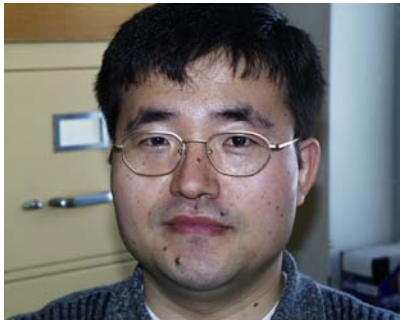
Antiferromagnetism vs d-wave superconductivity: Insights from the organics



B. Kyung, A.-M. Tremblay,
Université de Sherbrooke

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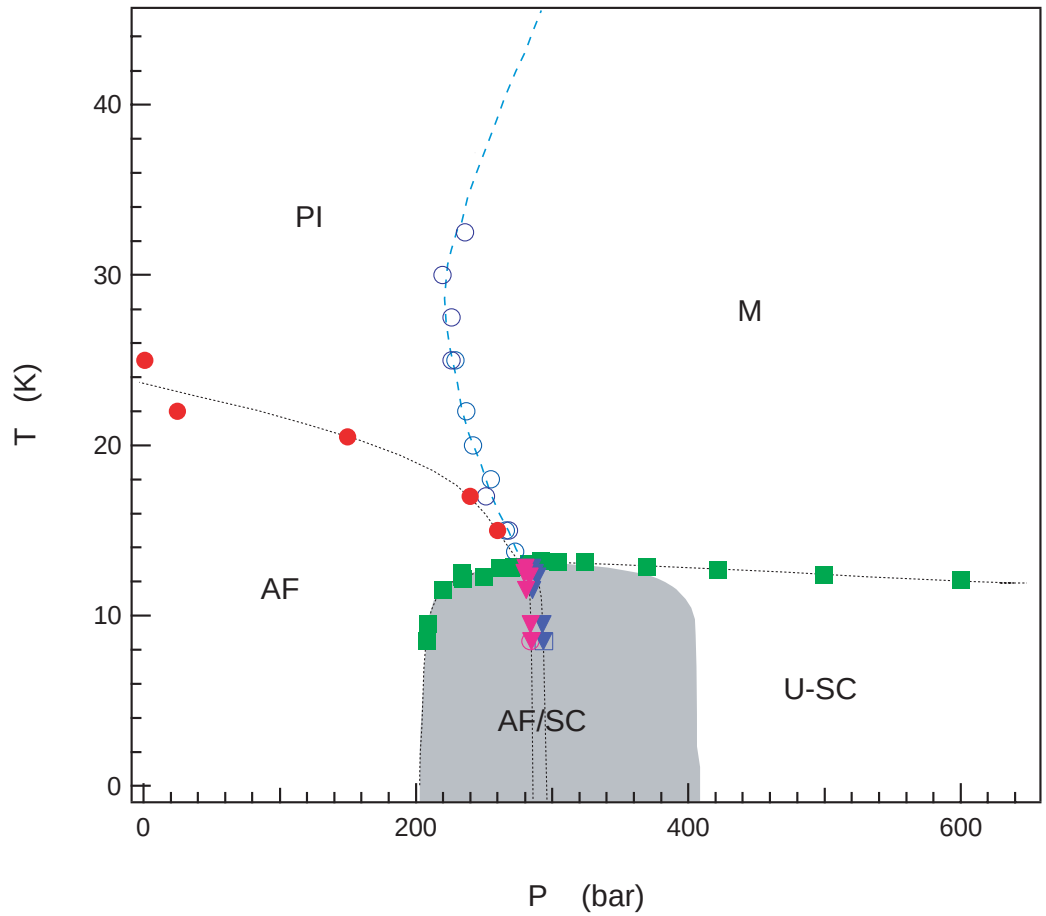
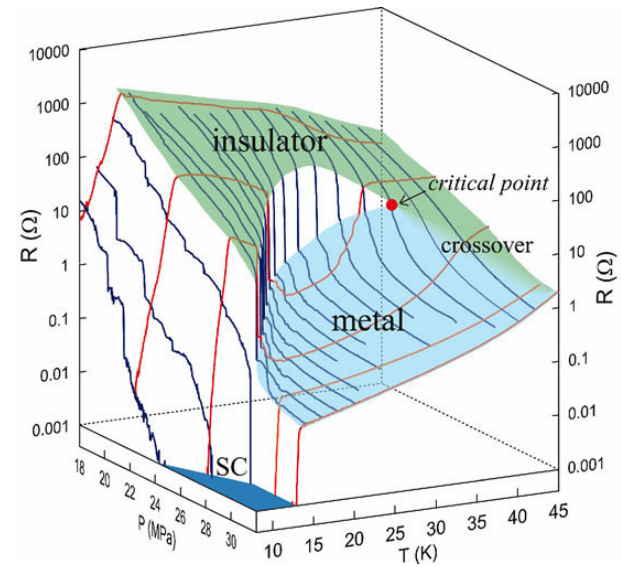
Motivation

Experimental phase diagram for κ- BEDT X





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

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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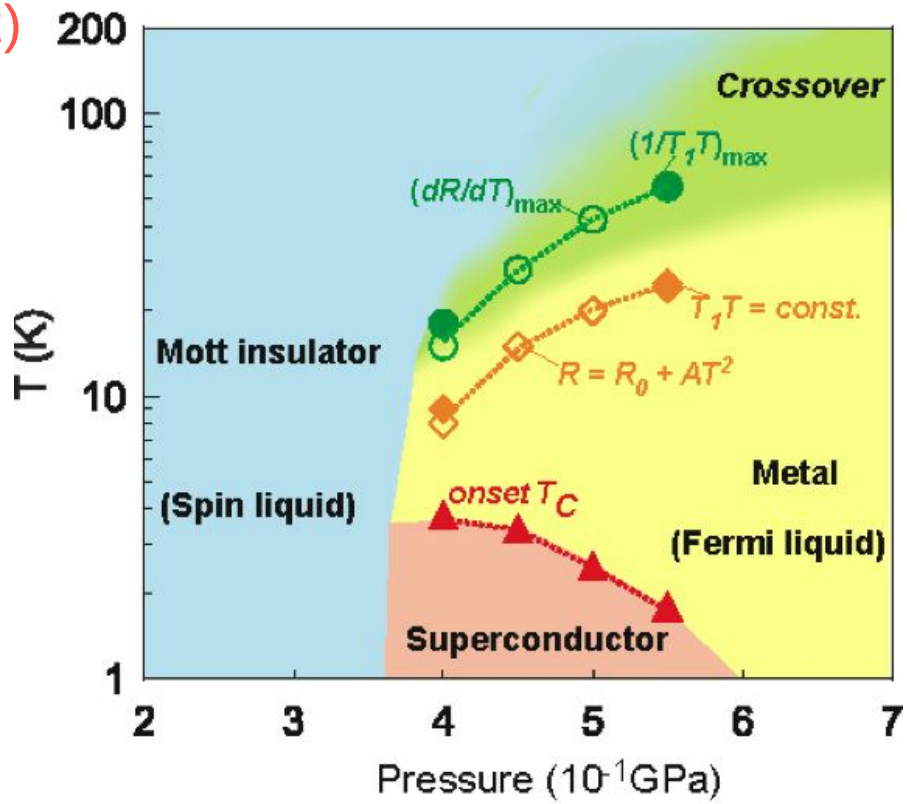
Proposal for AFM mediated d-wave superconductivity

- J. Schmalian PRL **81**, 4232 (’98);
- Kino + Kotani, JPSJ **67**,3691 (’98),
- Kondo + Moriya, JPSJ **67**,3695 (’98)
- M. Vojta +E. Dagotto, PRB, **59**, 713 (’99)

A spin liquid?

X= $Cu_2(CN)_3$ (t'~ t)



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

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

References on layered organics

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

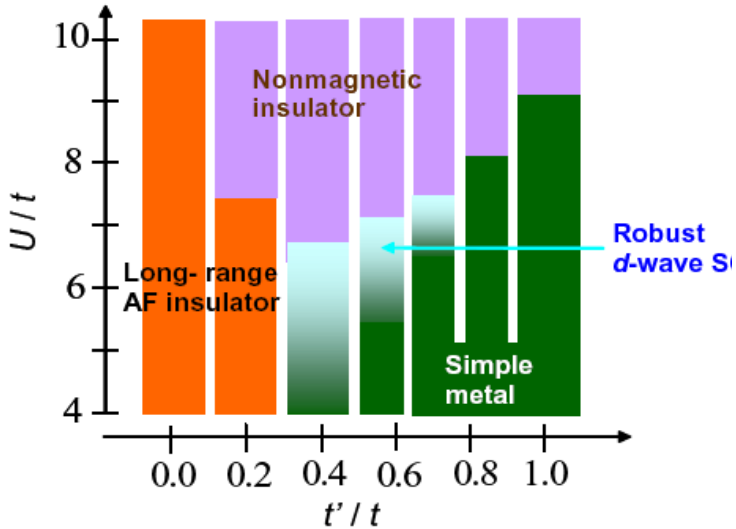
J. Liu, J. Schmalian, et al., Phys. Rev. Lett. 94, 127003 (2005). (VQMC)

S.S. Lee, P.A. Lee, Phys. Rev. Lett. 95, 036403 (2005). (U(1) gauge)

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

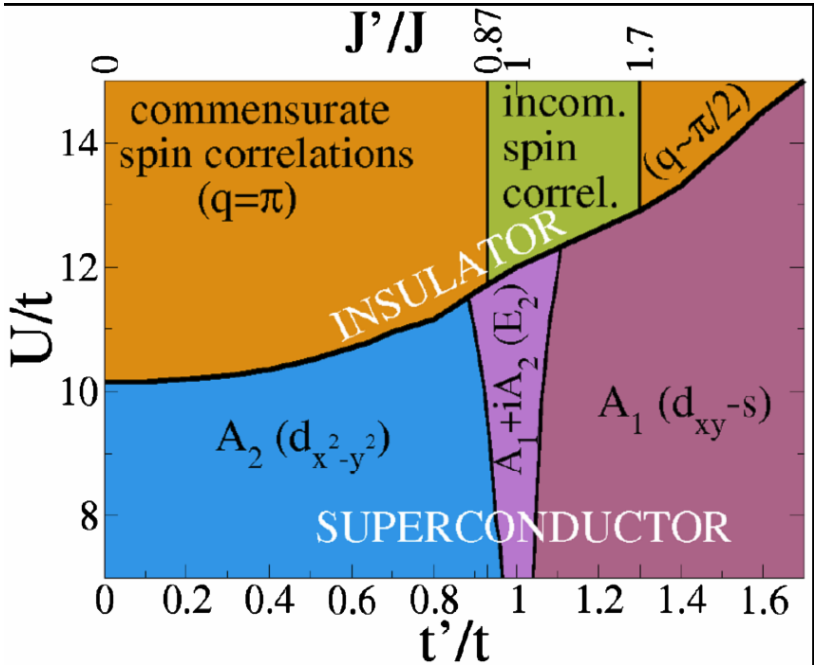
J.Y. Gan et al., Phys. Rev. Lett. 94, 067005 (2005). (Gossamer)

T. Watanabe et al., J. Phys. Soc. Japan **75,** 074707 (2006). (VQMC)

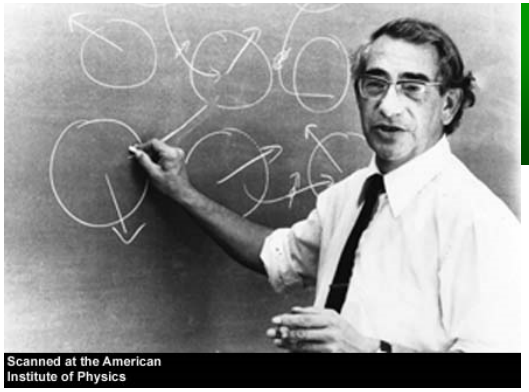


Recent issues

•Powell BJ, McKenzie RH
PRL **98,** 027005 (2007).



•Lee SS, Lee PA, Senthil T, PRL **98**, 067006 (2007).
-Amperean pairing instability in the U(1) spin liquid state
•V. Galitski, Y.-B. Kim
- Spin-triplet pairing instability

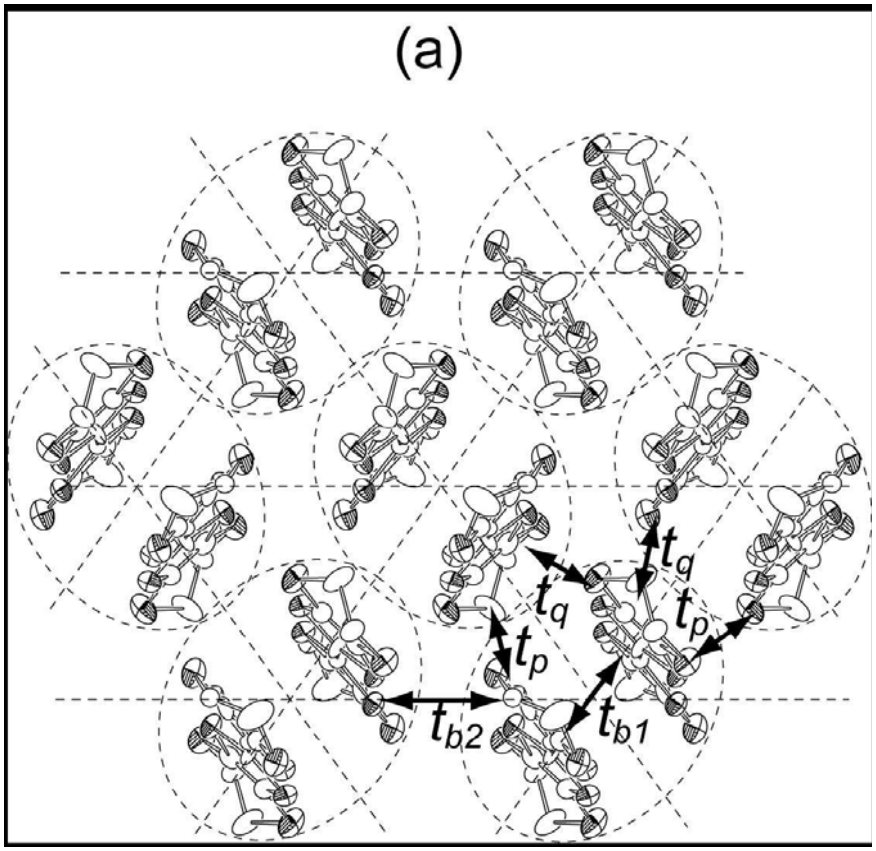


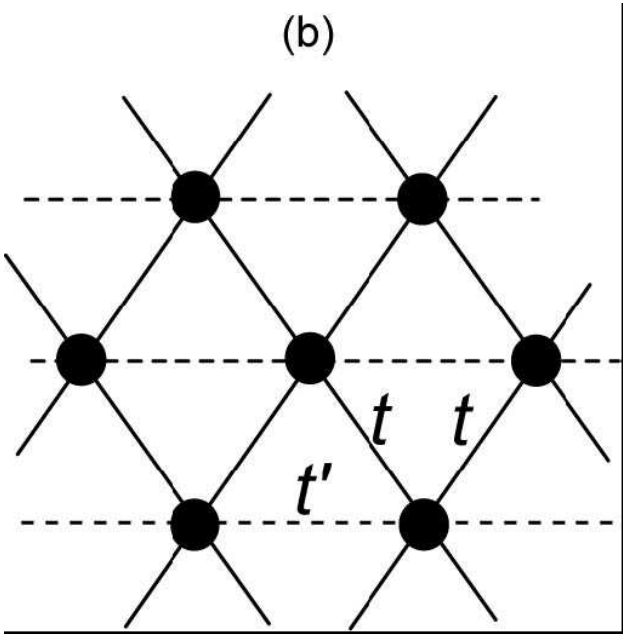
One-band Hubbard model

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

One-band Hubbard model for BEDT organics

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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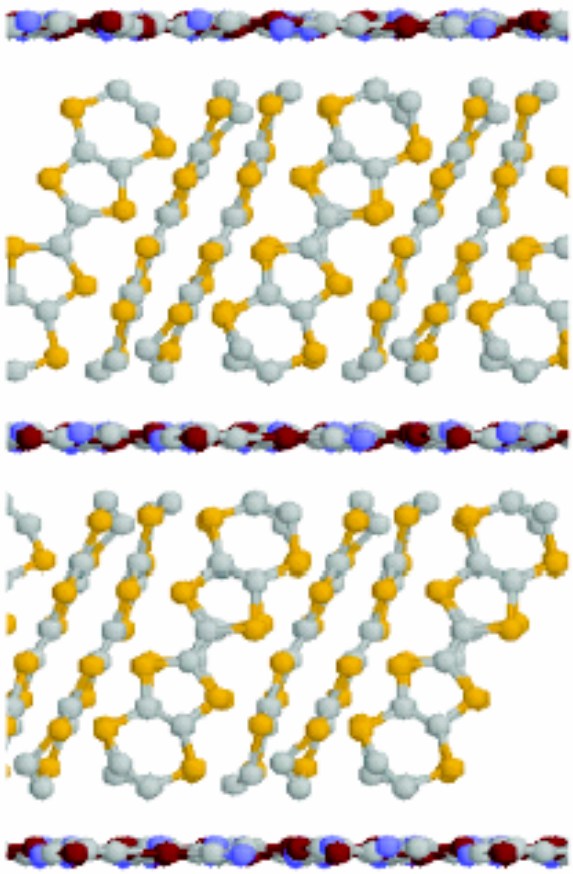
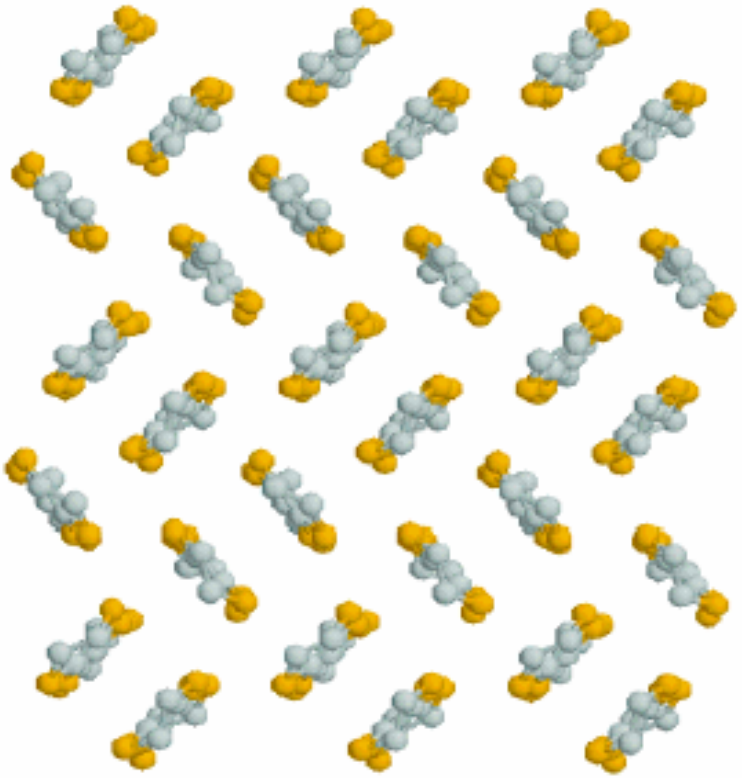
Layered organics (κ–BEDT-X family)

BEDT-TTF layer

Anion layer

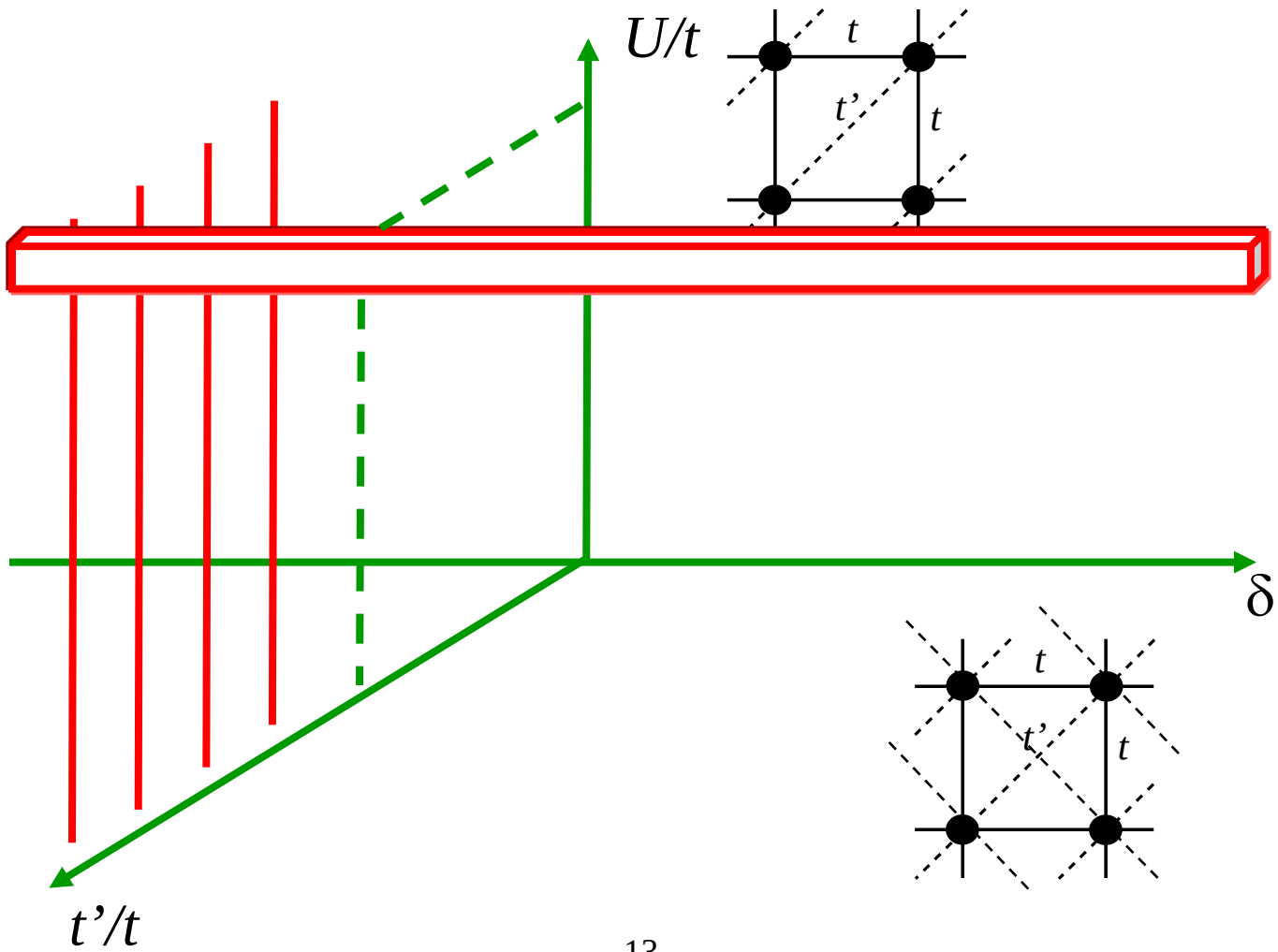
(*t'* / *t*)





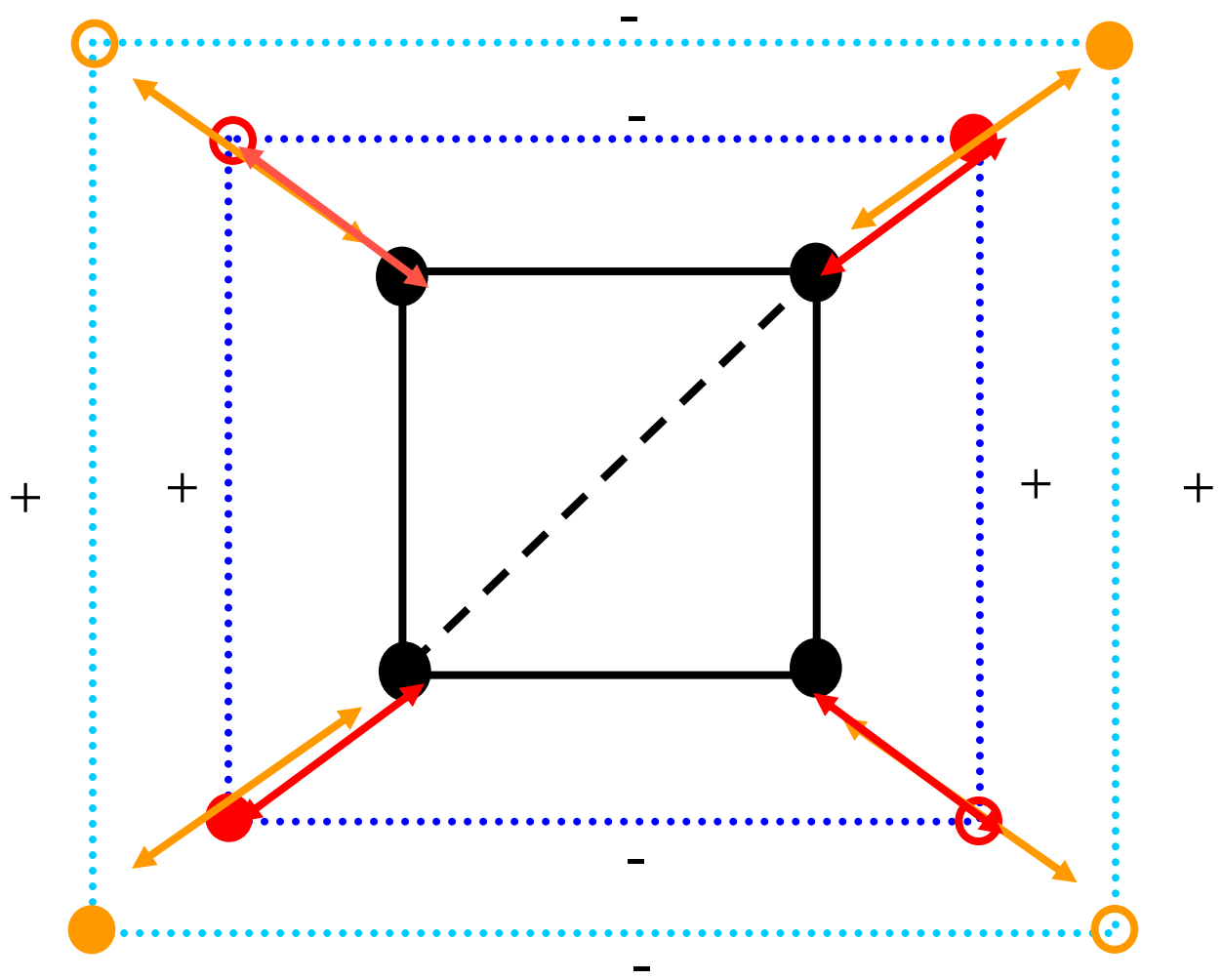
n = 1

Perspective



Methodology

CDMFT + ED



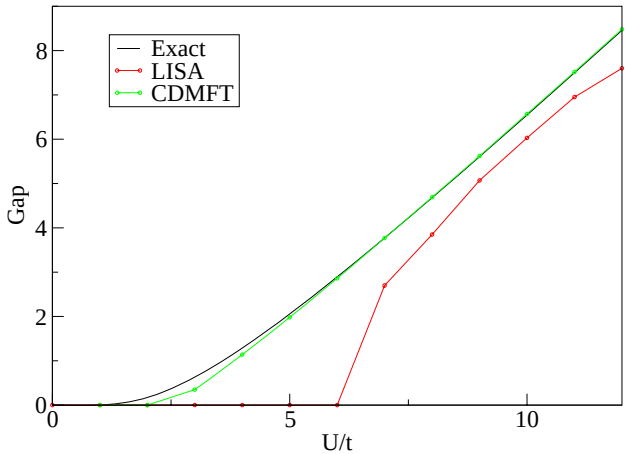
Savrasov, Kotliar, PRB (2001)

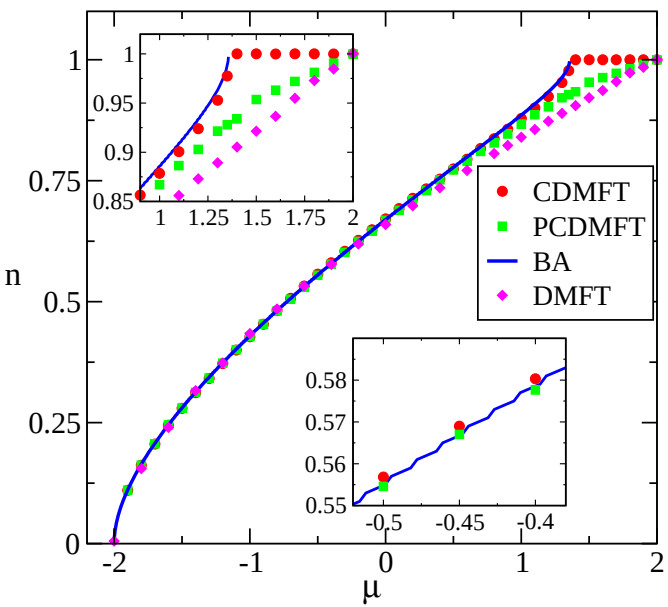
Caffarel and Krauth, PRL (1994)

No Weiss field on the cluster!

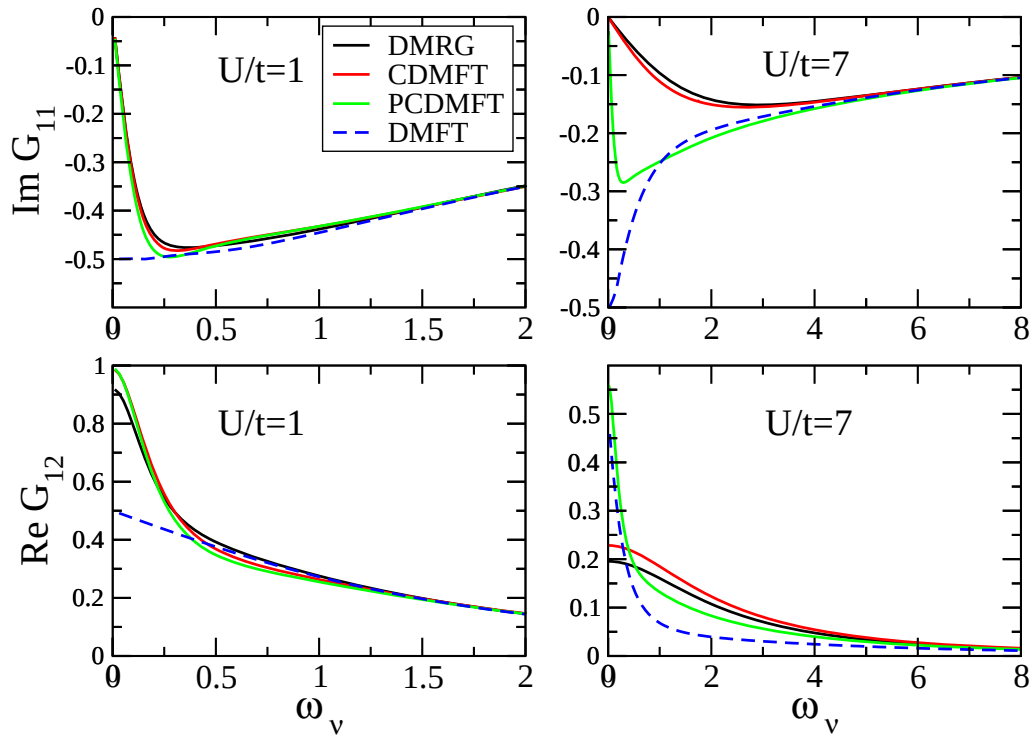
U is never factorized

Tests : CDMFT





1D Hubbard model: Worst case scenario



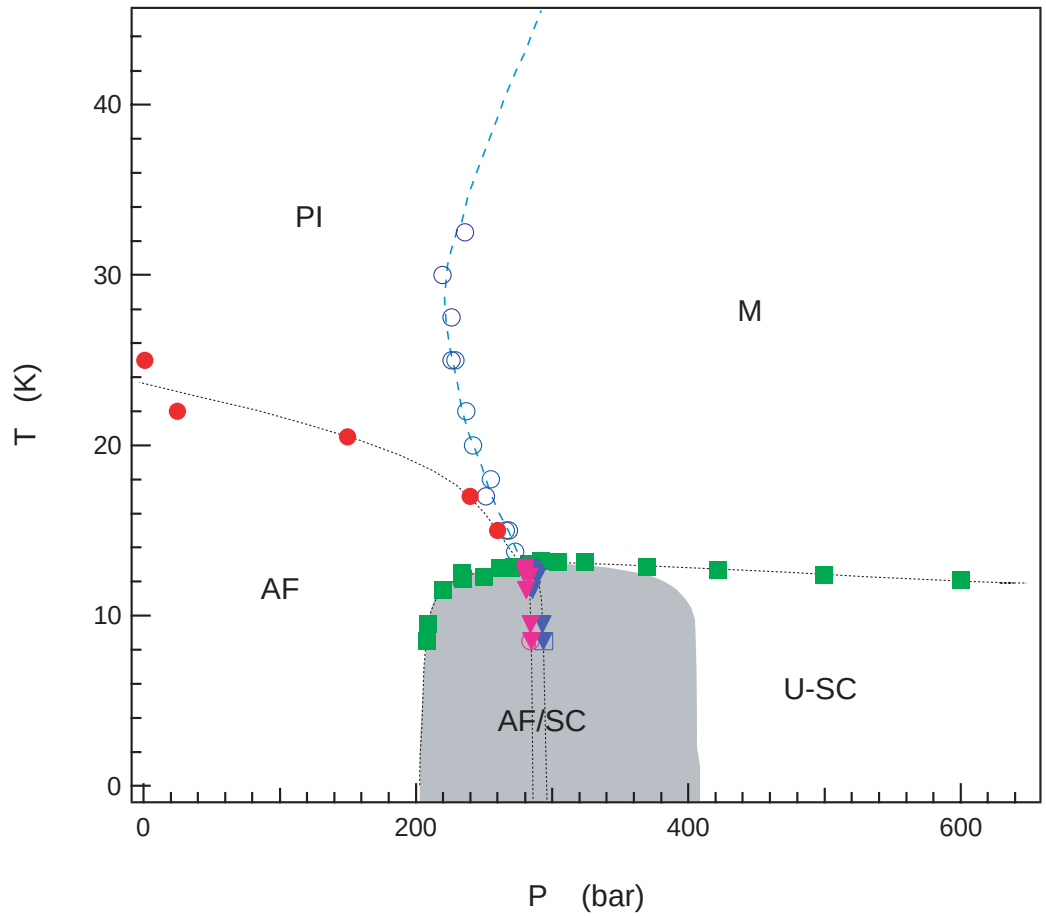
Excellent agreement with exact results in both metallic and insulating limits

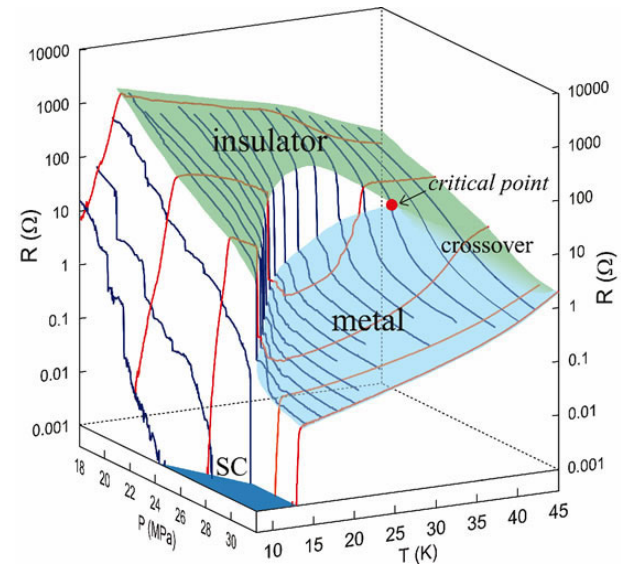
Capone, Civelli, SSK, Kotliar, Castellani PRB (2004)

Bolech, SSK, Kotliar PRB (2003)

Results

Experimental phase diagram for Cl anions





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

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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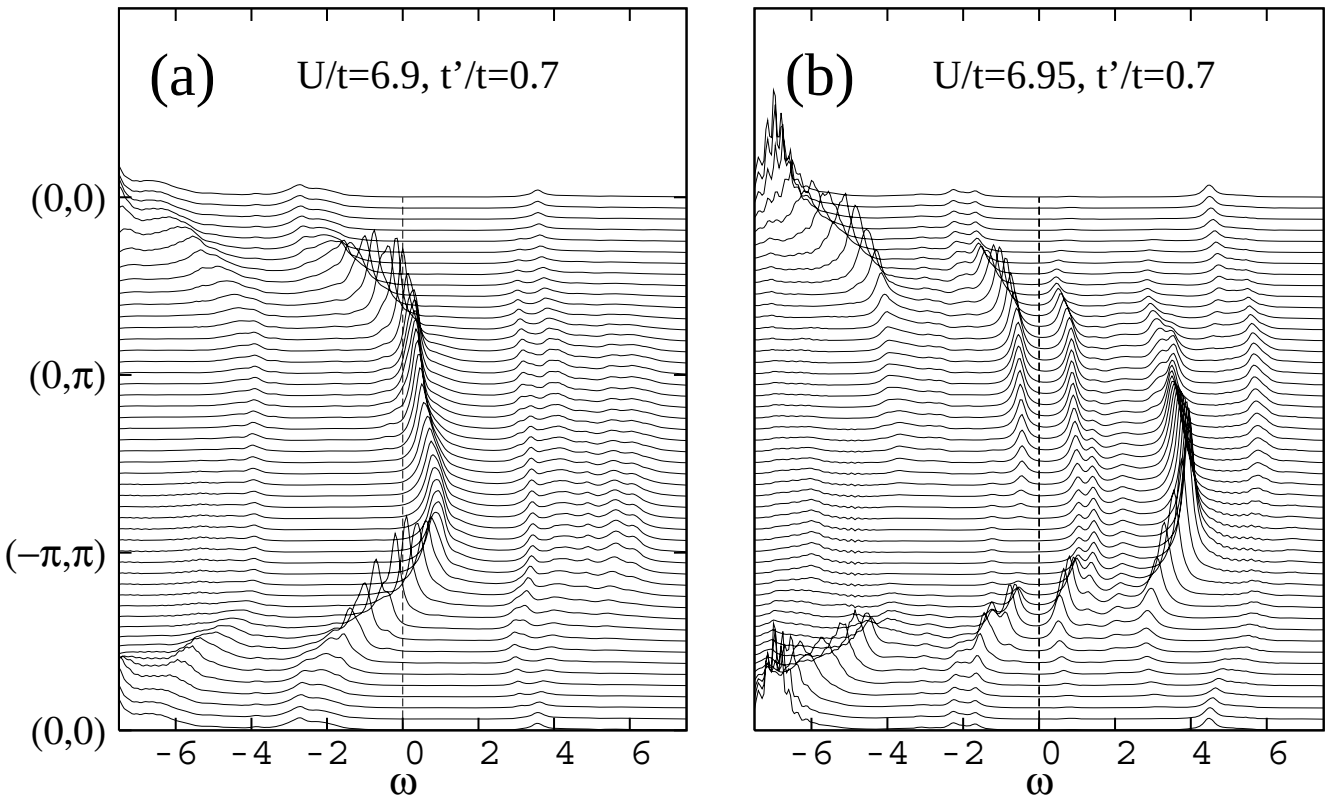
Mott transition (C-DMFT)



Kyung, A.-M.S.T. PRL (2006)

See also, Sénéchal, Sahebsara, PRL (2006)

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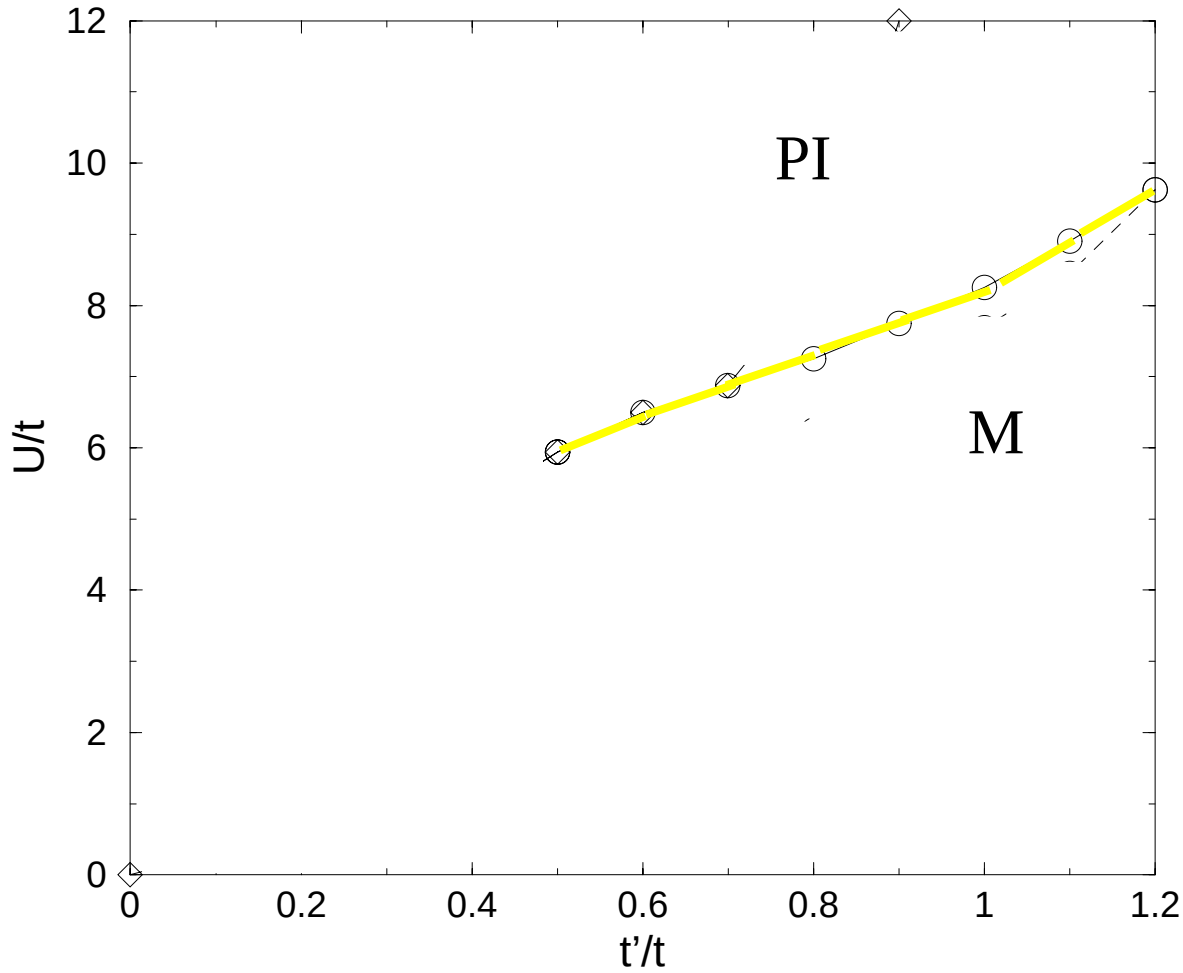
Normal phase theoretical results for BEDT-X



Kyung, A.-M.S.T. PRL (2006)

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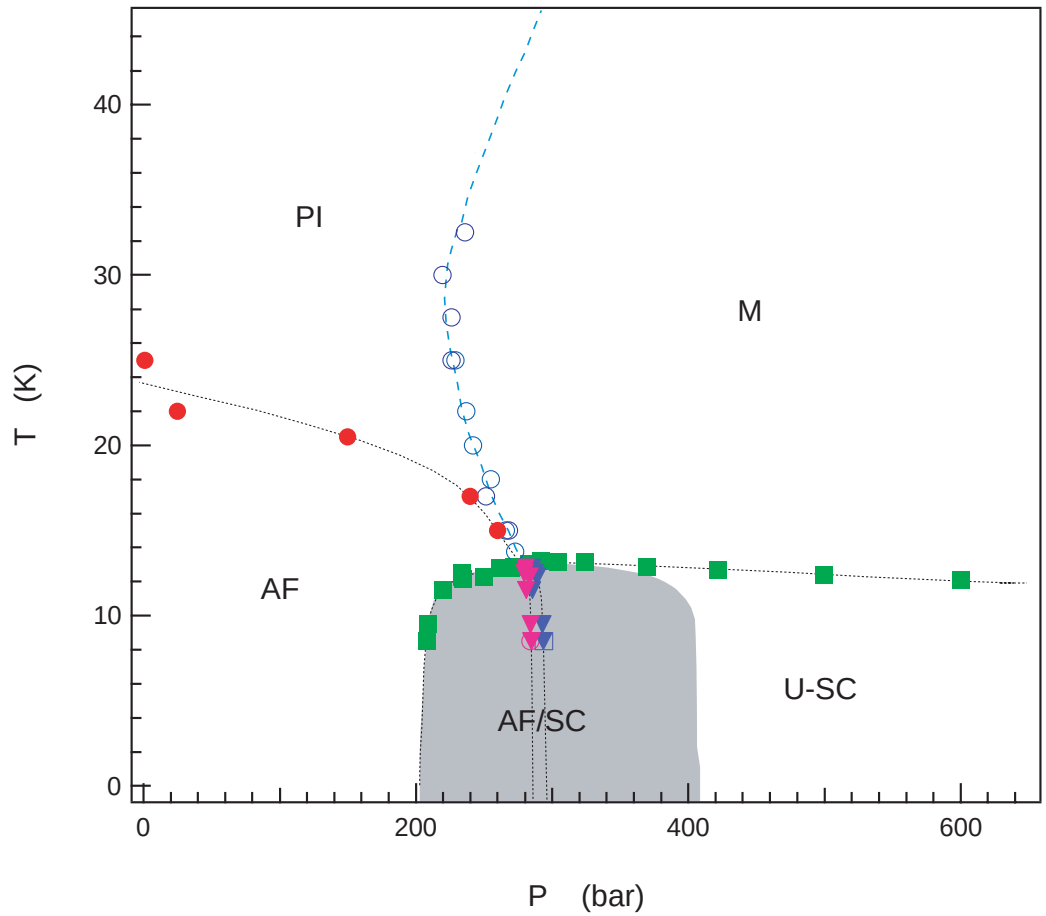
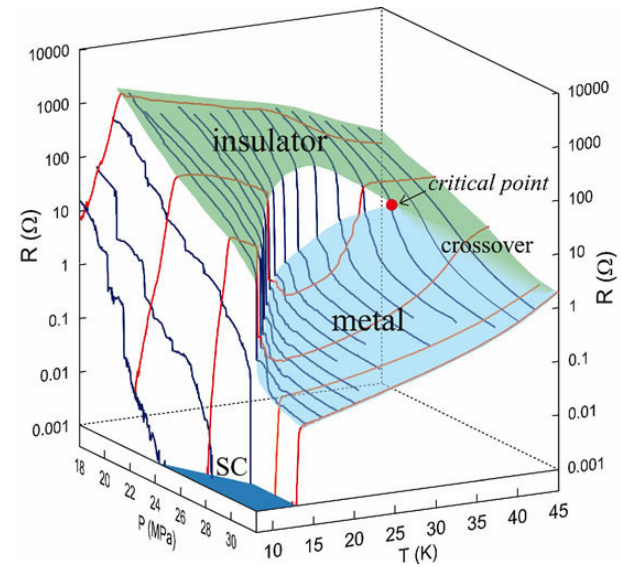
Experimental phase diagram for Cl anion





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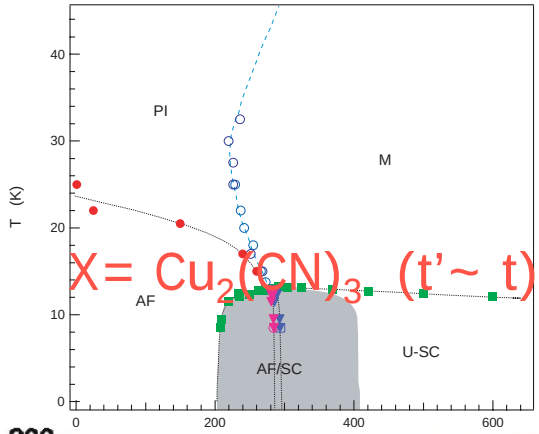
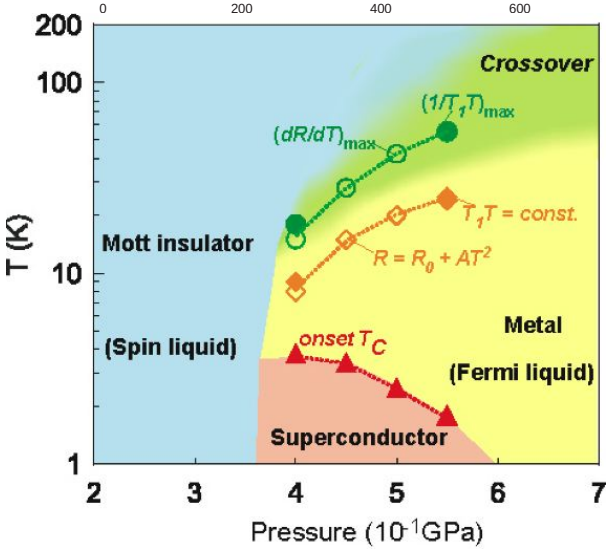
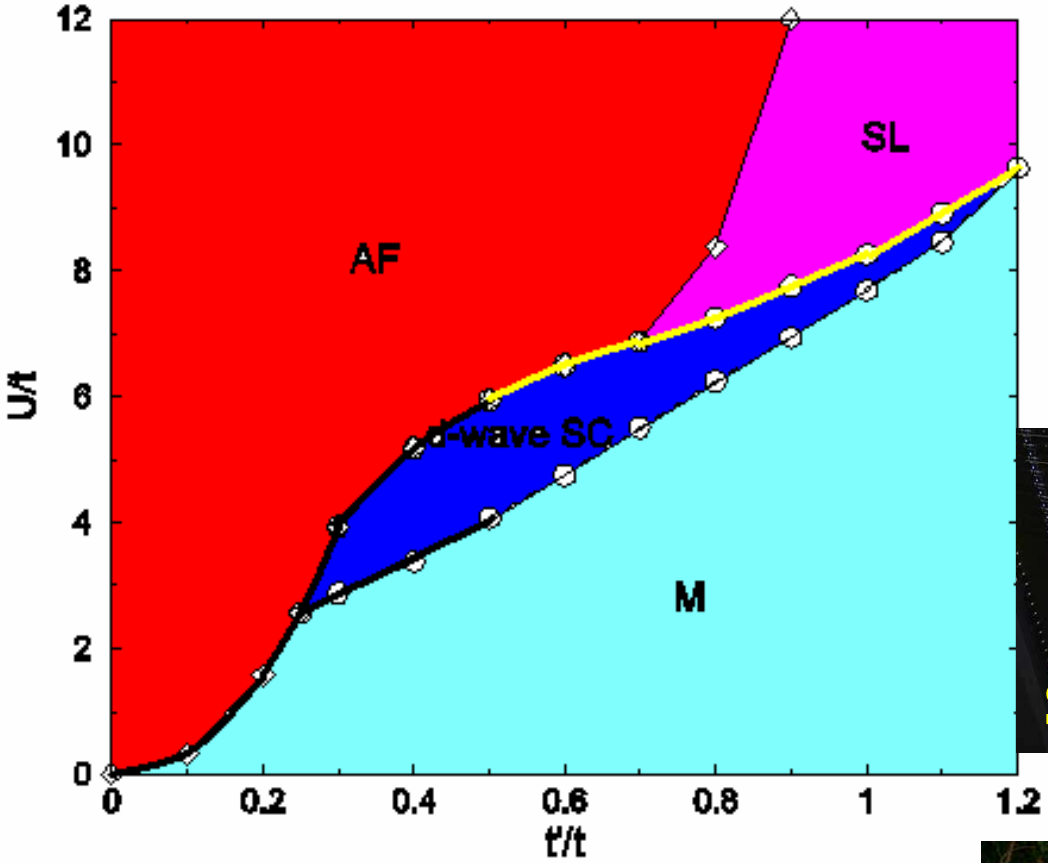
Theoretical phase diagram BEDT





Y. Kurisaki, et al.

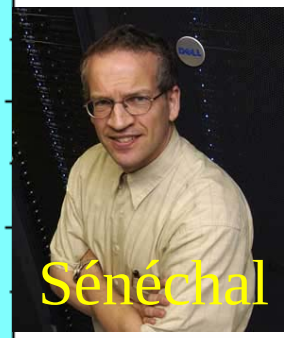
Phys. Rev. Lett. **95**, 177001(2005)



Kyung, A.-M.S.T. PRL (2006)

Sénéchal, Sahebsara, PRL 97, 257004 (2006)

OP



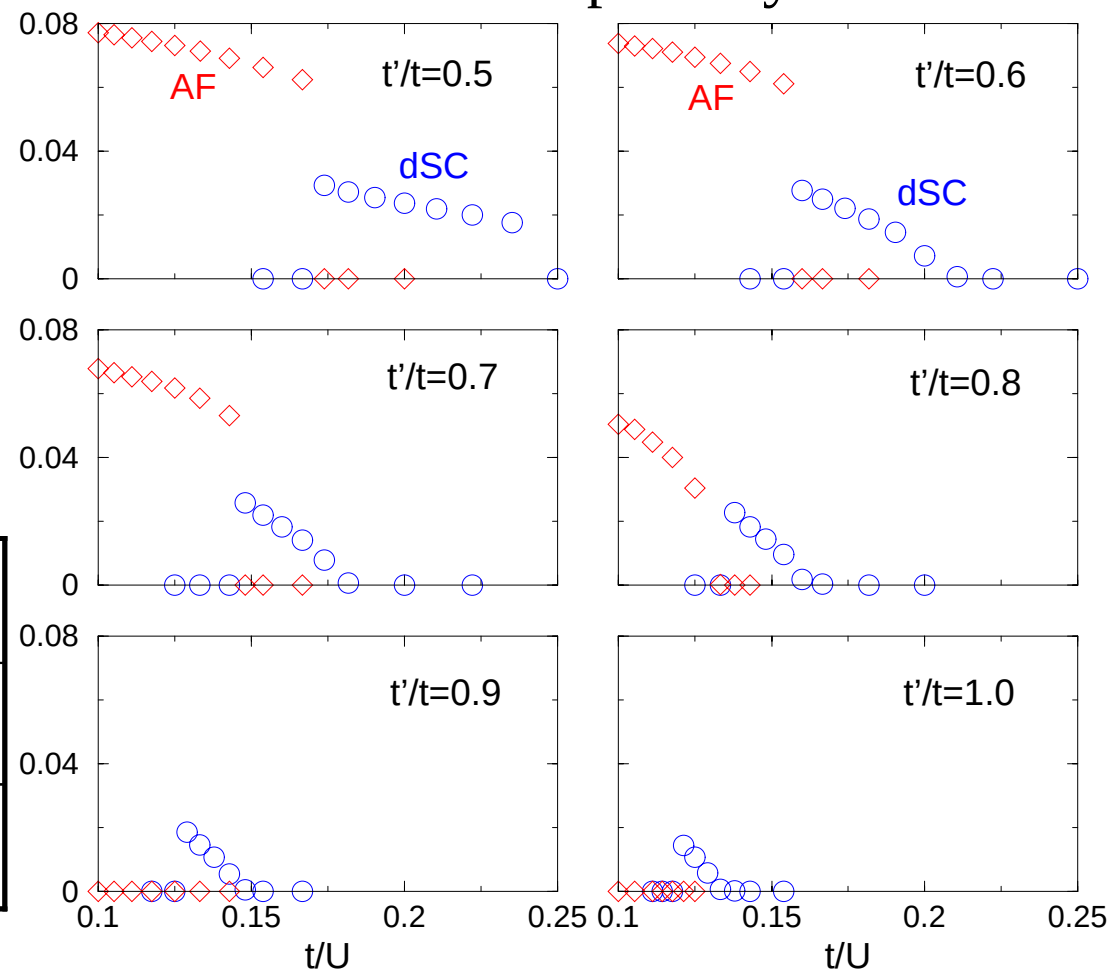
Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

AFM and dSC order parameters for various t'/t

- Discontinuous jump
- Correlation between maximum order parameter and Tc

X	$Cu[N(CN)_2]Br$	$Cu(NCS)_2$	$Cu_2(CN)_3$
t'/t	0.68	0.84	1.06
T_c	11.6	10.4	3.9

AF multiplied by 0.1



Kyung, A.-M.S.T. PRL **97**, 046402 (2006)

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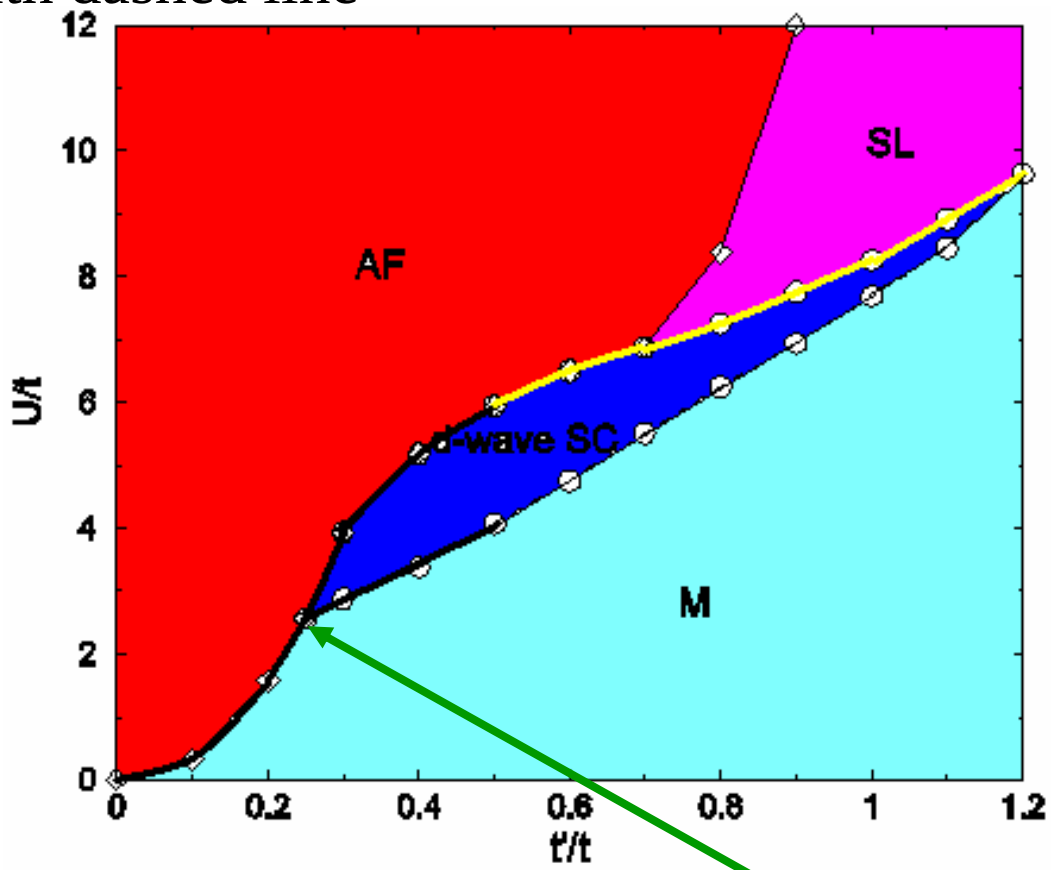
d-wave

•All transitions first order, except one with dashed line



Kyung, A.-M.S.T. PRL **97**, 046402 (2006)

Sénéchal, Sahebsara, PRL **97**, 257004 (2006)

•Triple point, not *SO(5)*

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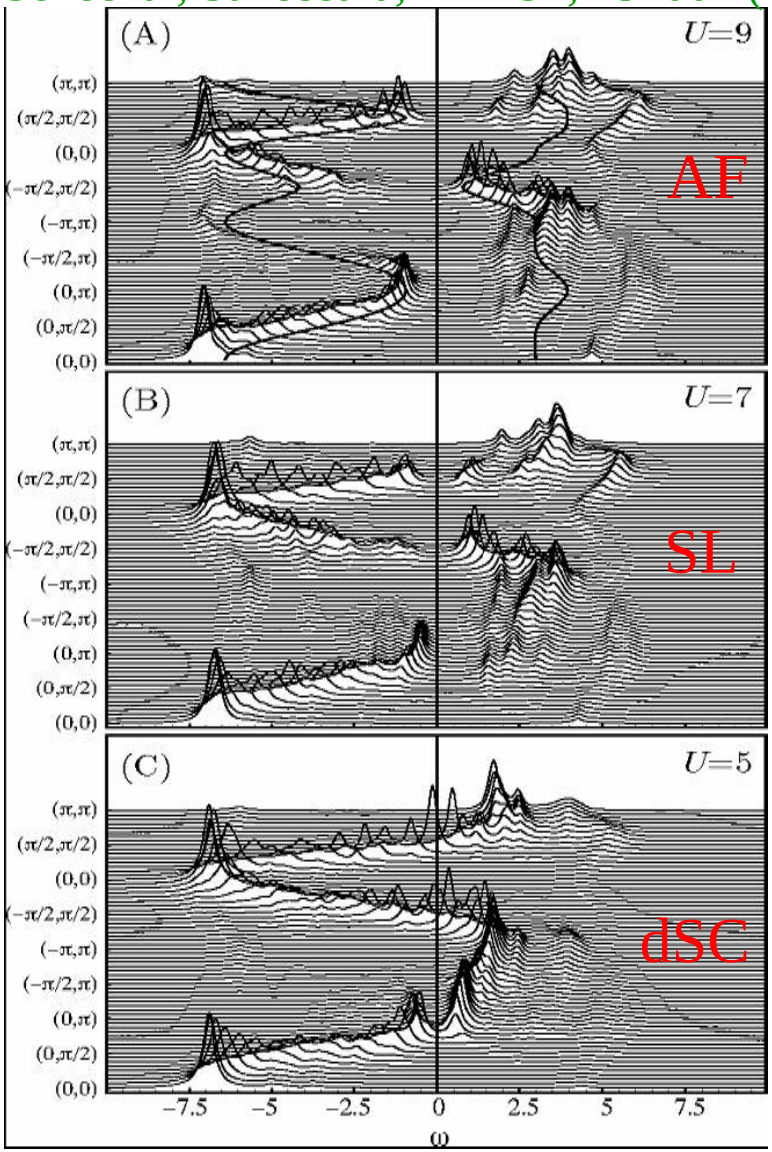
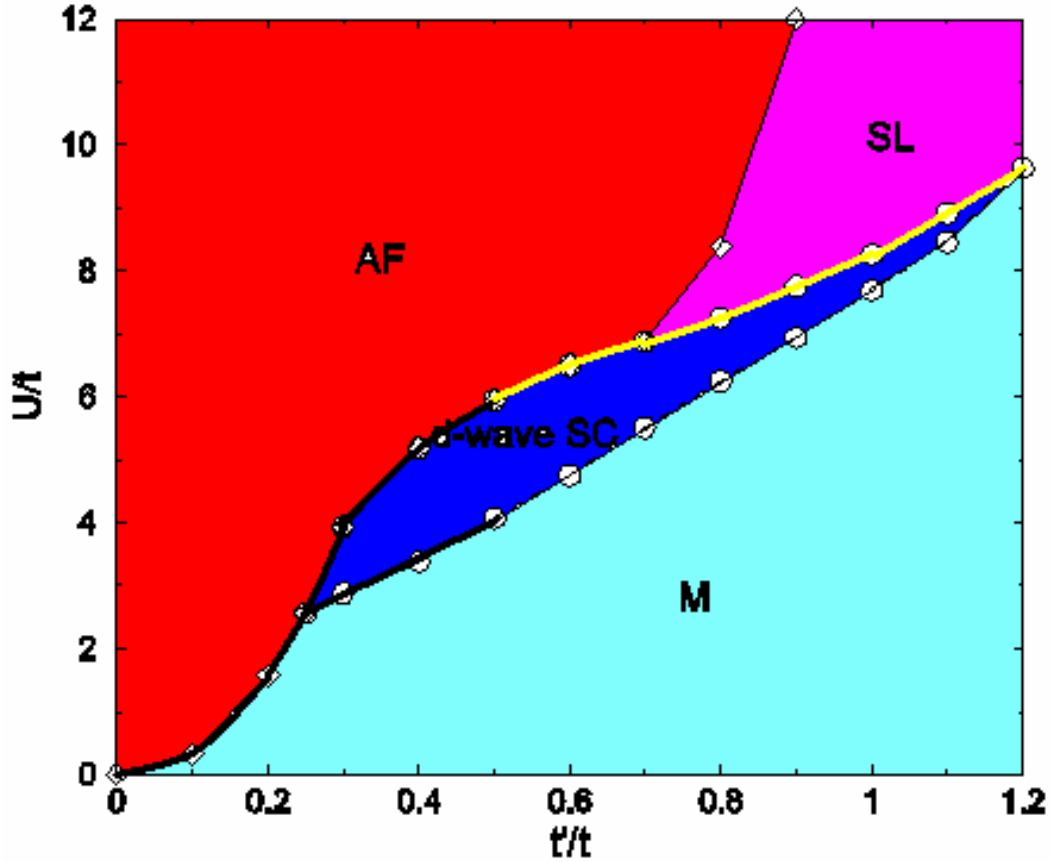
Prediction of a new type of pressure behavior

Sénéchal, Sahebsara, PRL 97, 257004 (2006)

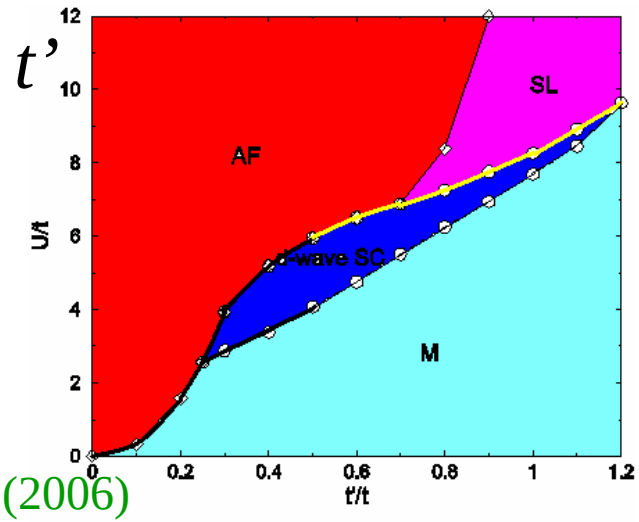


Kyung, A.-M.S.T. PRL (2006)



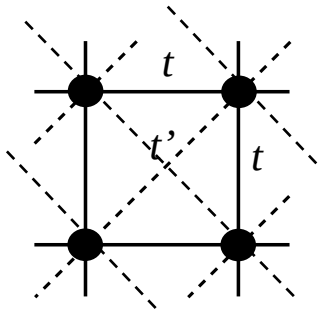
Conclusion

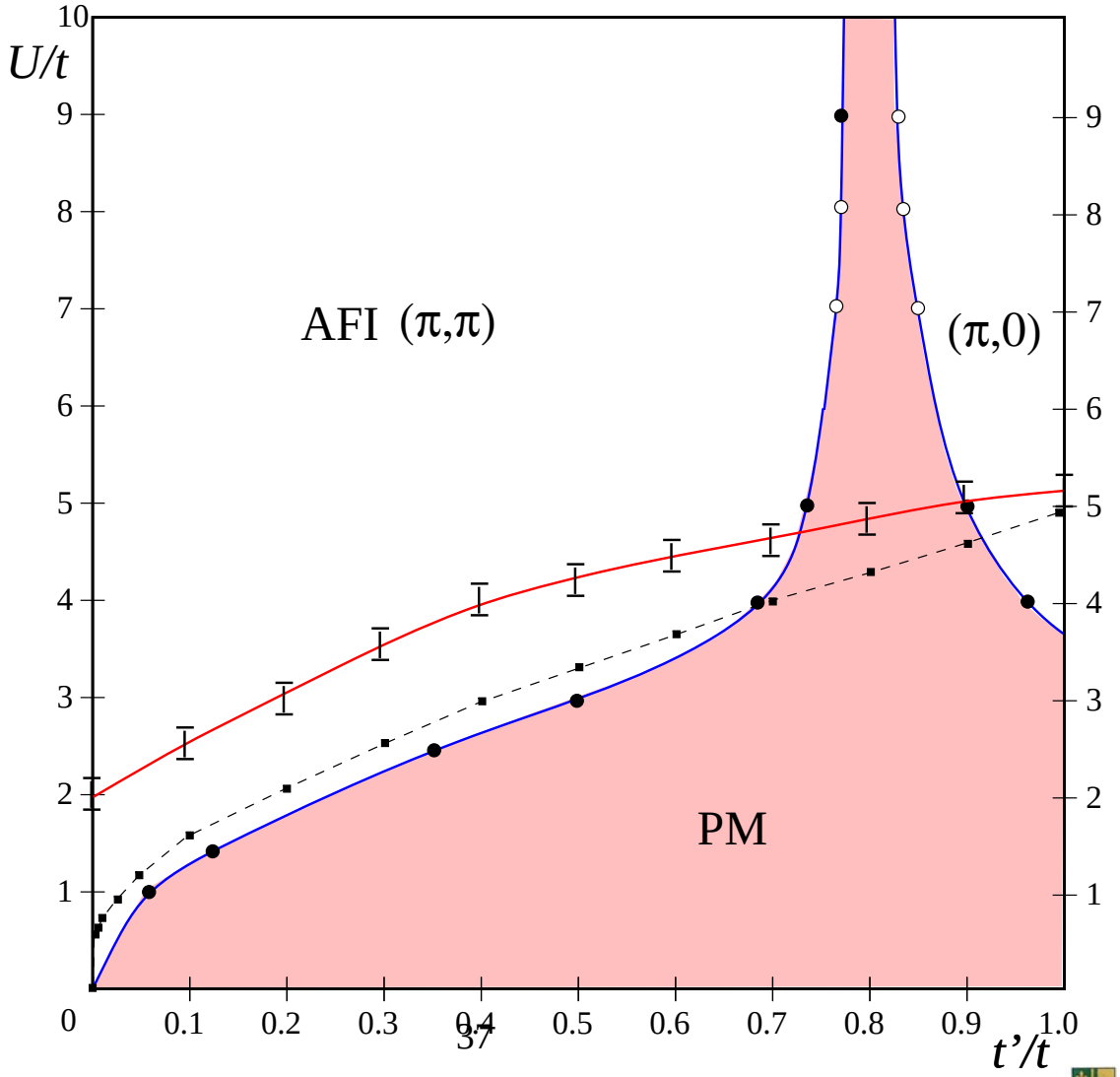
- One-band Hubbard model on anisotropic triangular lattice contains main experimental features of layered organics:
  - Mott transition in normal state
  - First-order transition between AFM and d-SC or between SL and d-SC depending on frustration
  - Order parameter largest at transition
  - d-SC order parameter decreases with *t'*
- Insights on d-SC, role of *t'* and *J*
- Correct methodology for High T_c



Kyung, A.-M.S.T. PRL **97**, 046402 (2006)

High-Tc lattice at half-filling





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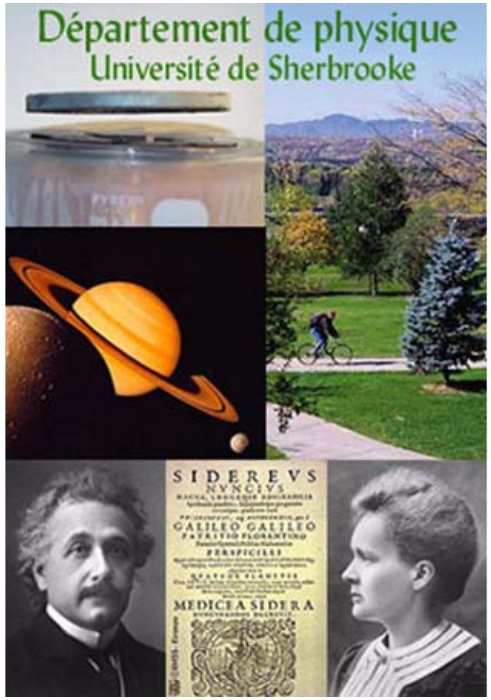
André-Marie Tremblay



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Thank you

Merci