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A unified perspective on cuprates and layered organic superconductors

A.-M.S. Tremblay,
Charles-David Hébert, Giovanni Sordi, Patrick Sémon

A62.00004, APS March Meeting Boston
Monday, March 4, 2019, BCEC Room: 258C
9:48 AM–10:24 AM

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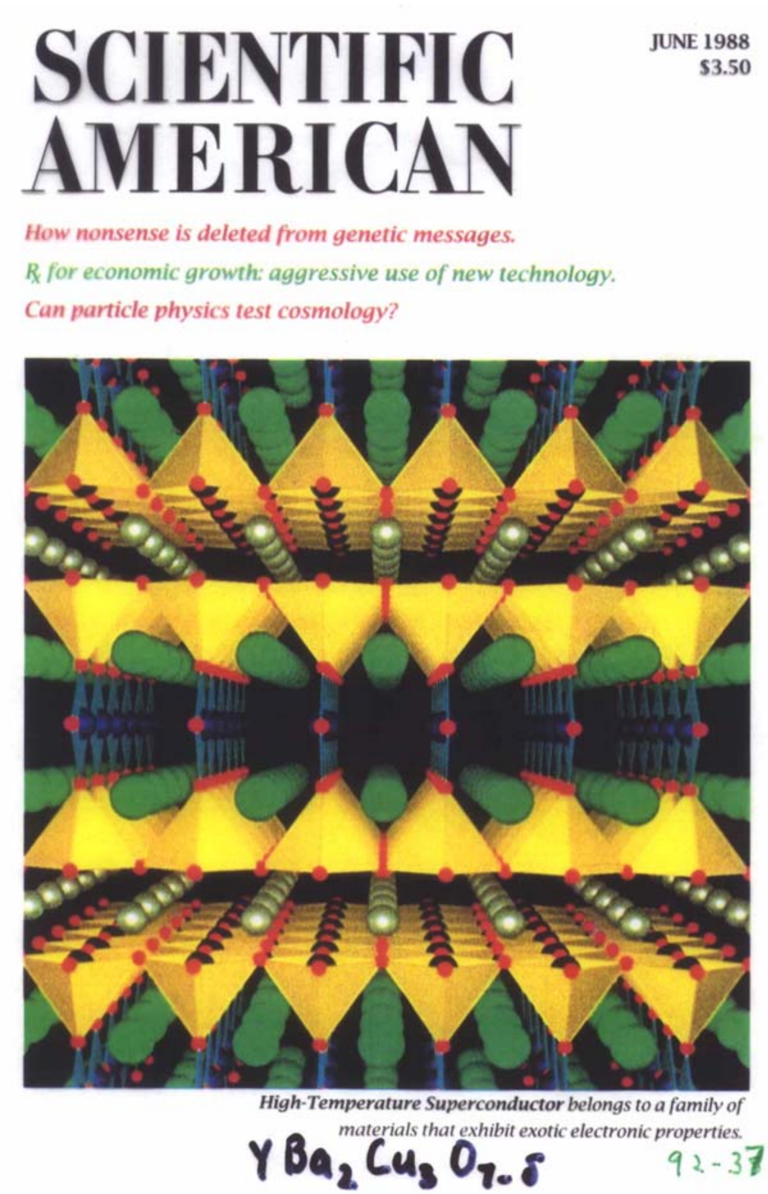
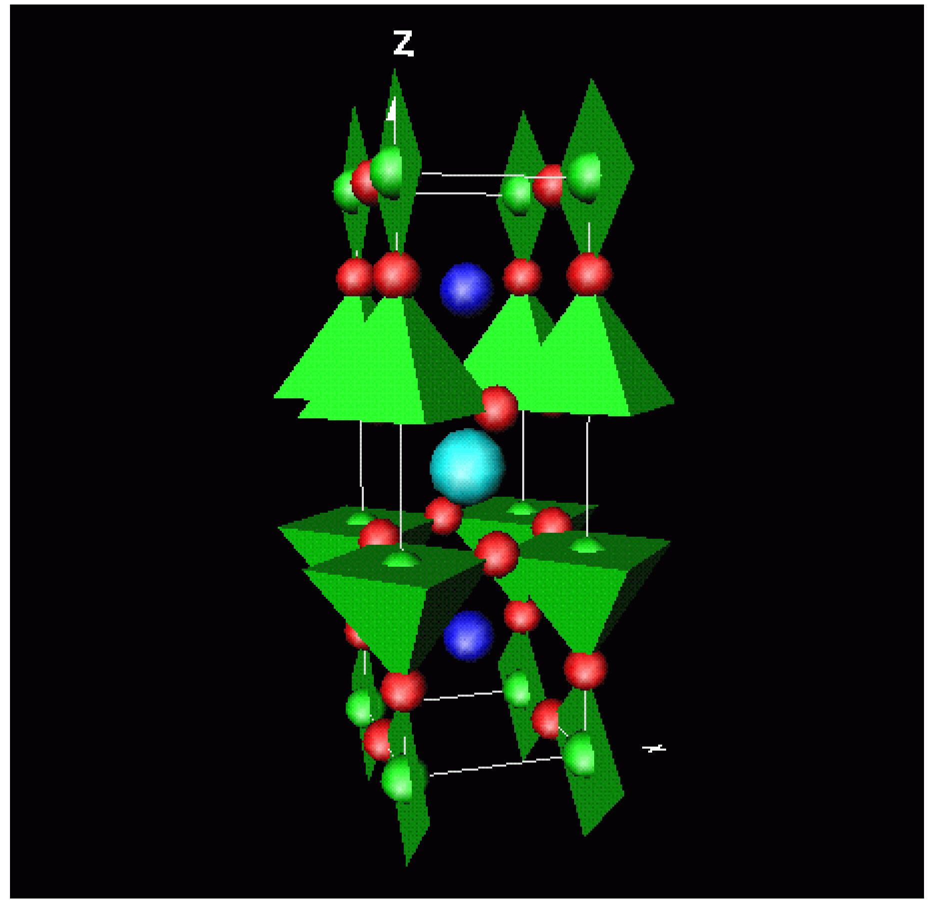
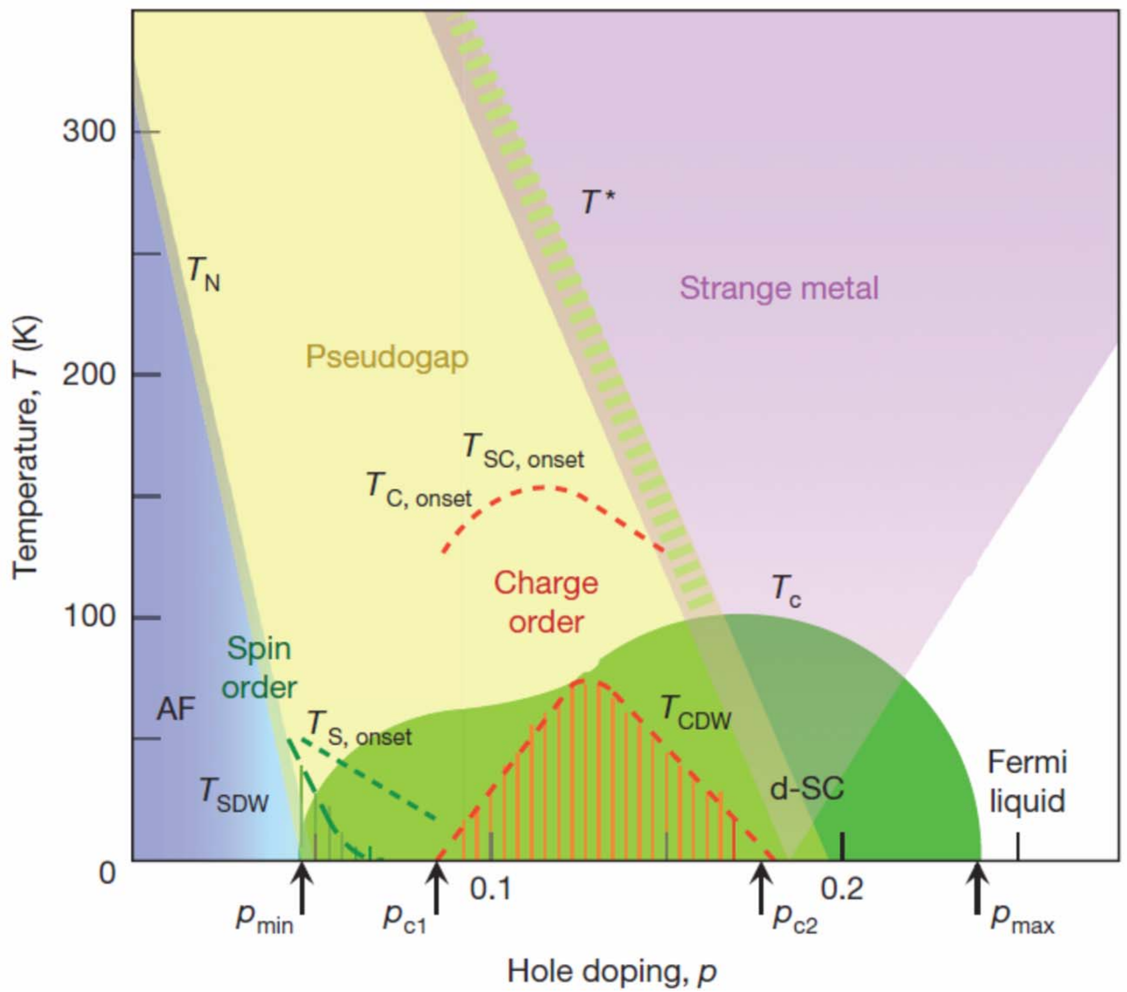
Atomic structure





Phase diagram $YBa_2Cu_3O_{7-x}$

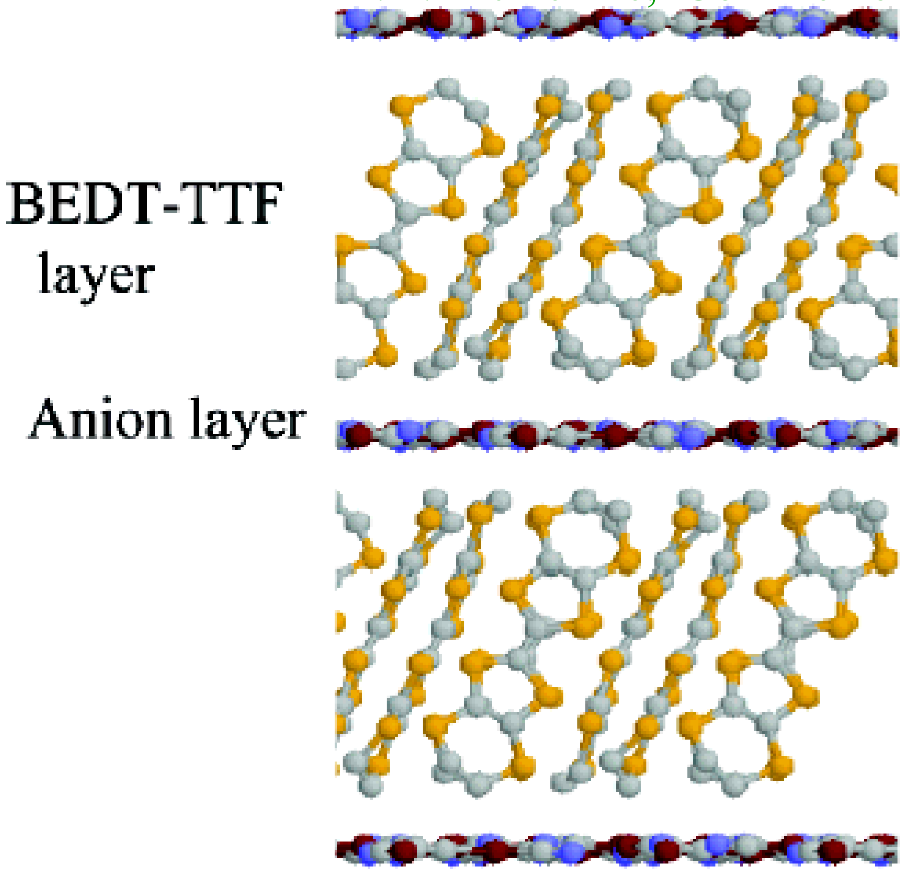


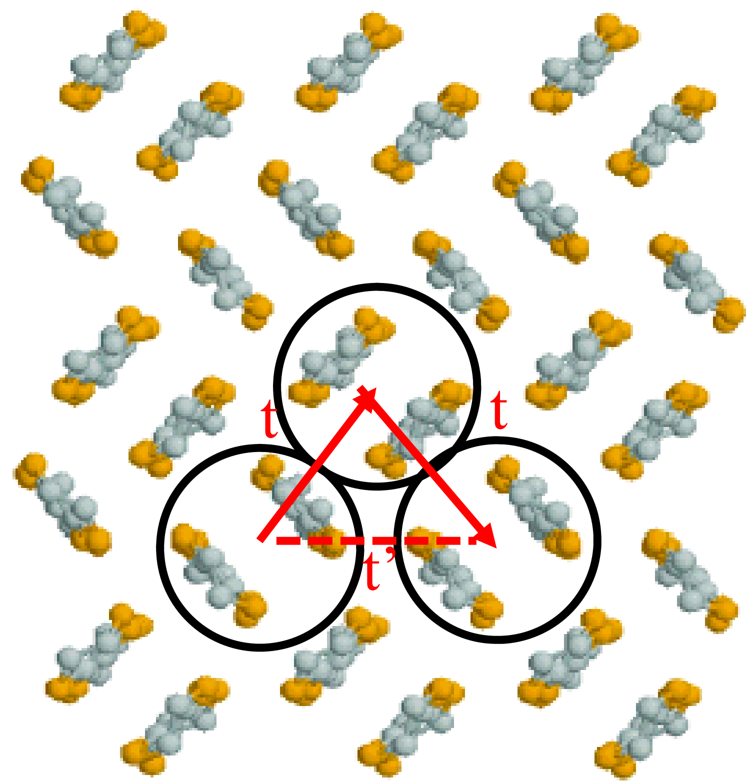
p or δ

Keimer et al., Nature 518, 179 (2015)

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)





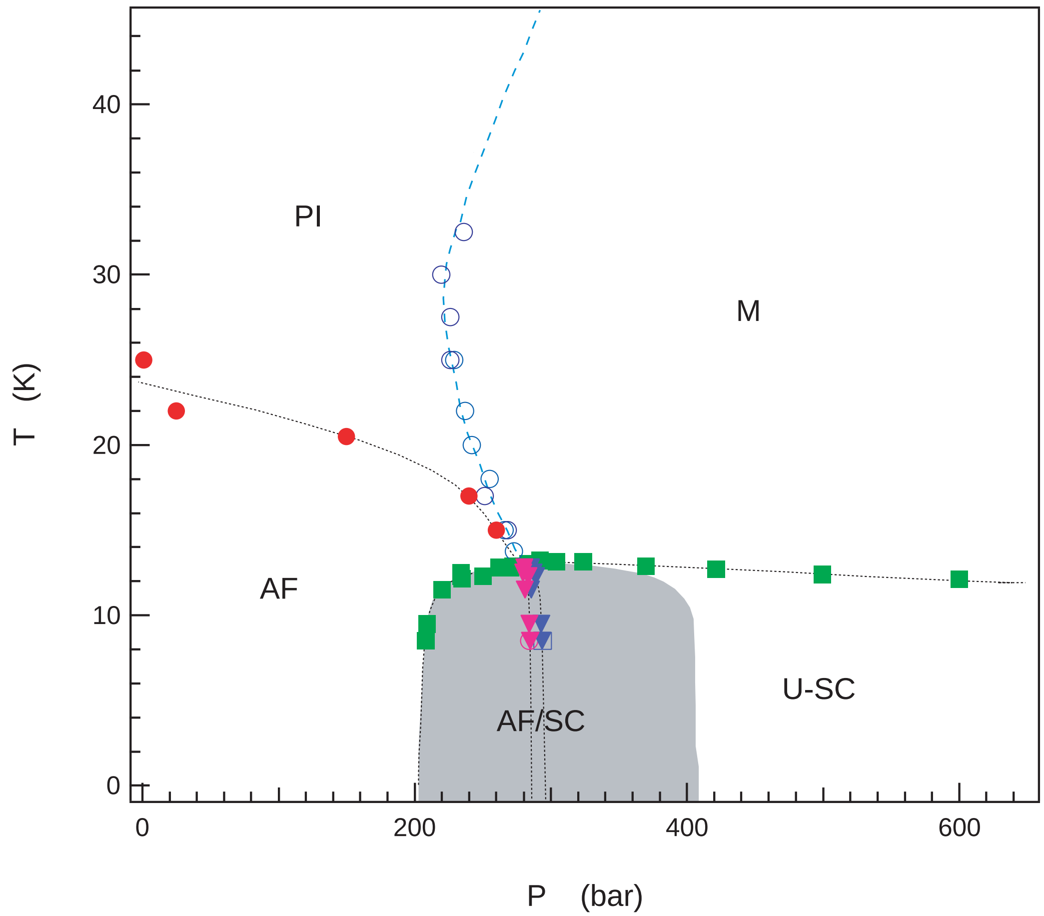
$$t \approx 50\,\text{meV}$$

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

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

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

Phase diagram for organics

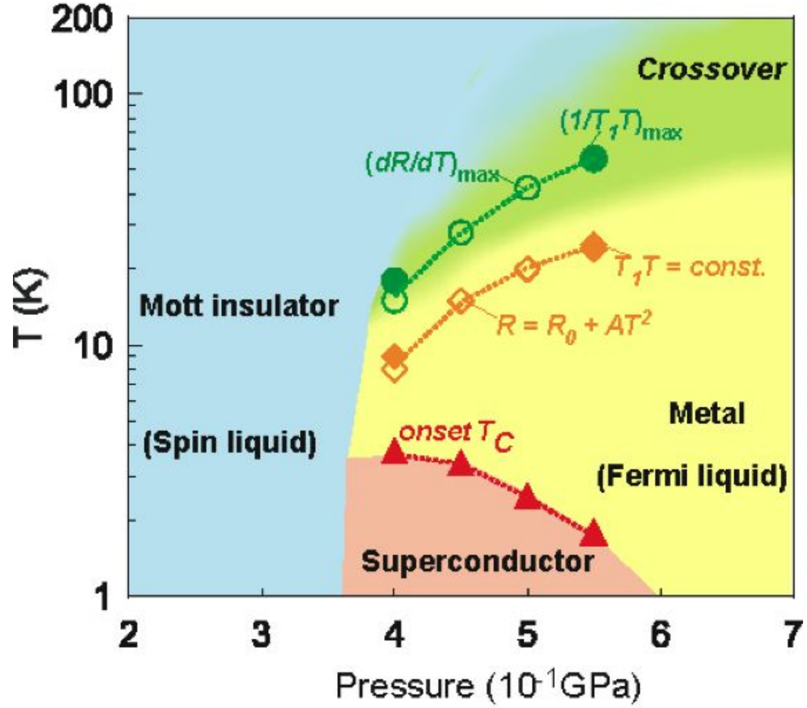


Phase diagram ($X=Cu[N(CN)_2]Cl$)

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

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)

Model

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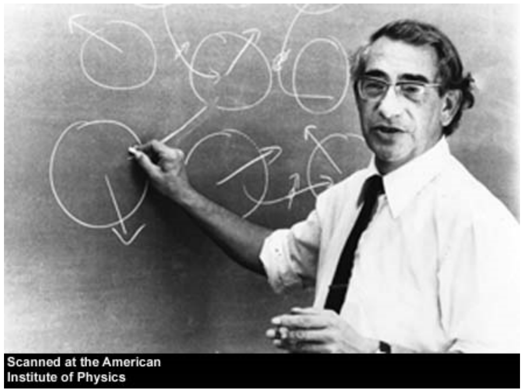
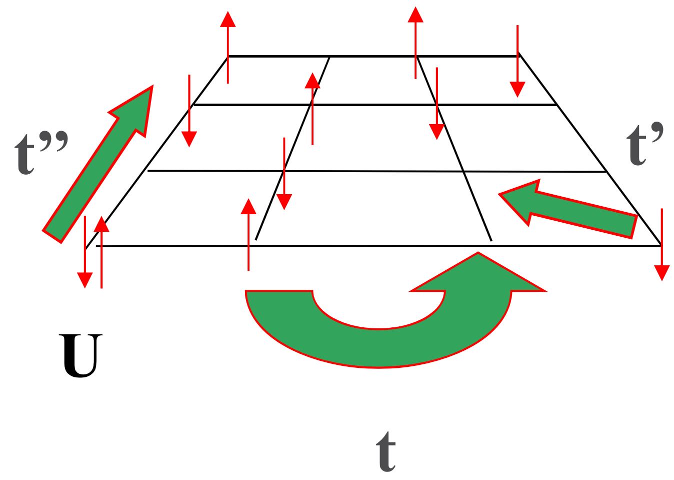
Hubbard Model



1931-1980

μ

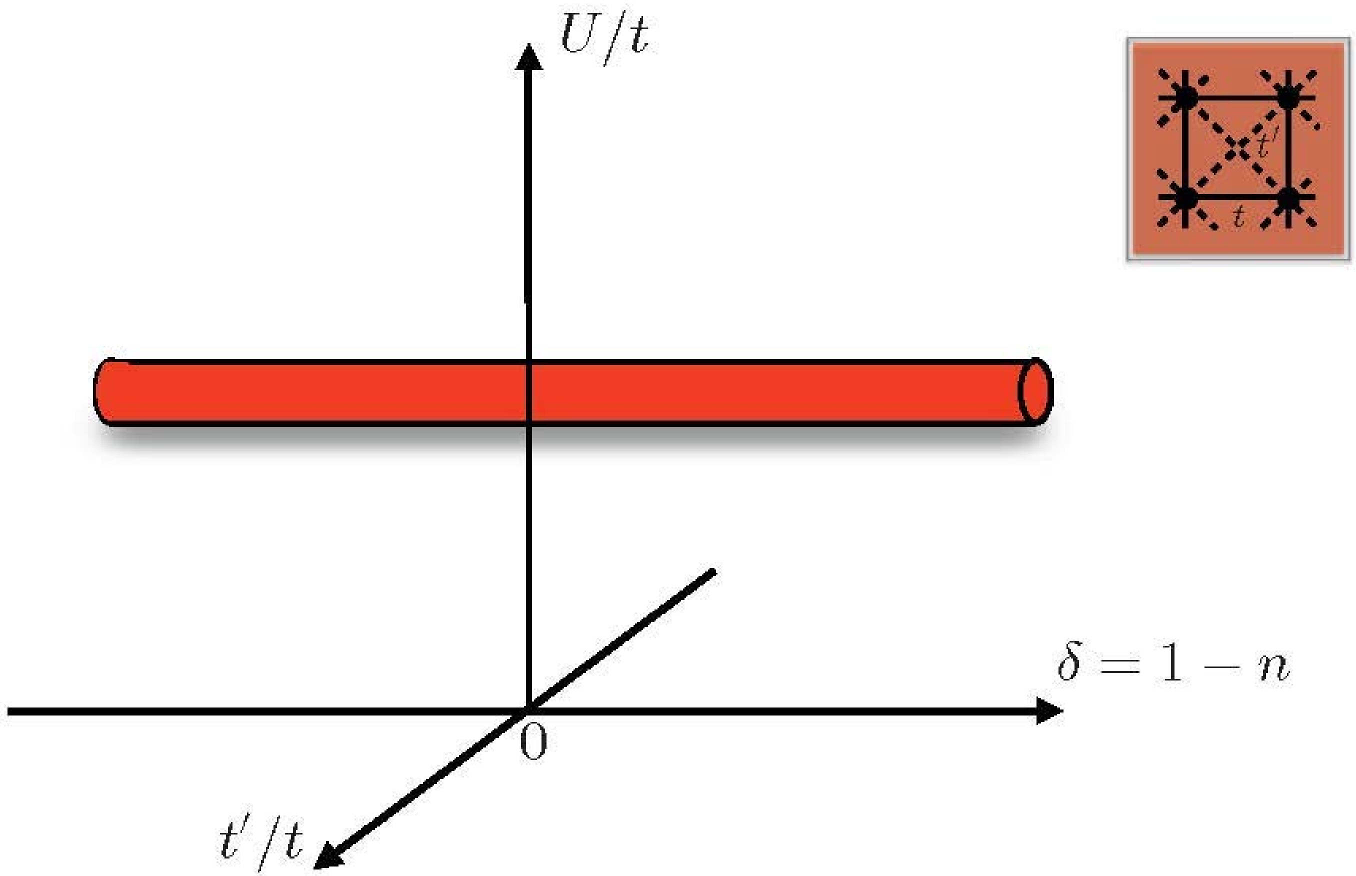


$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

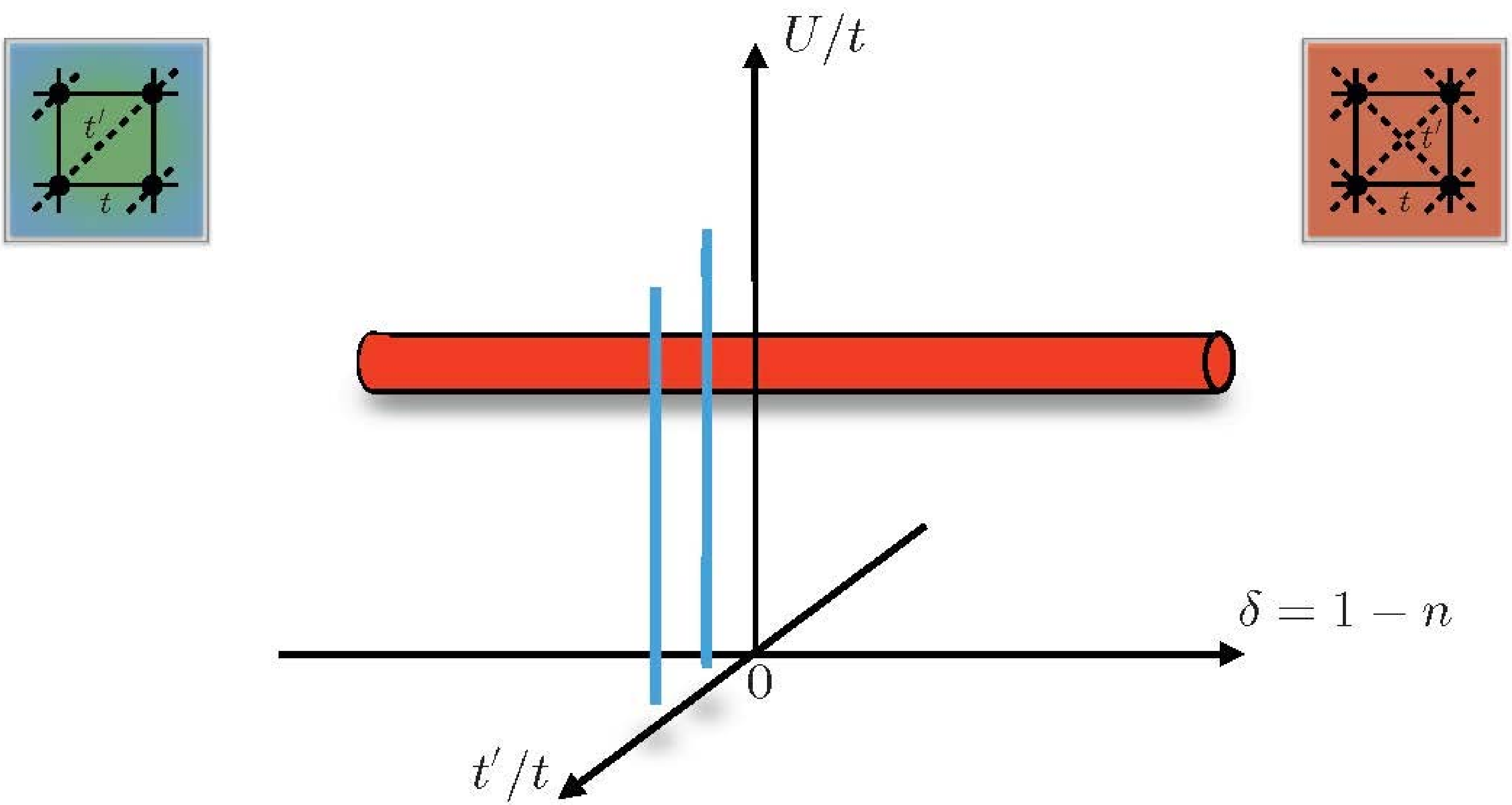
$$t = 1,\ k_B = 1,\ \hbar = 1$$

Attn: Charge transfer insulator

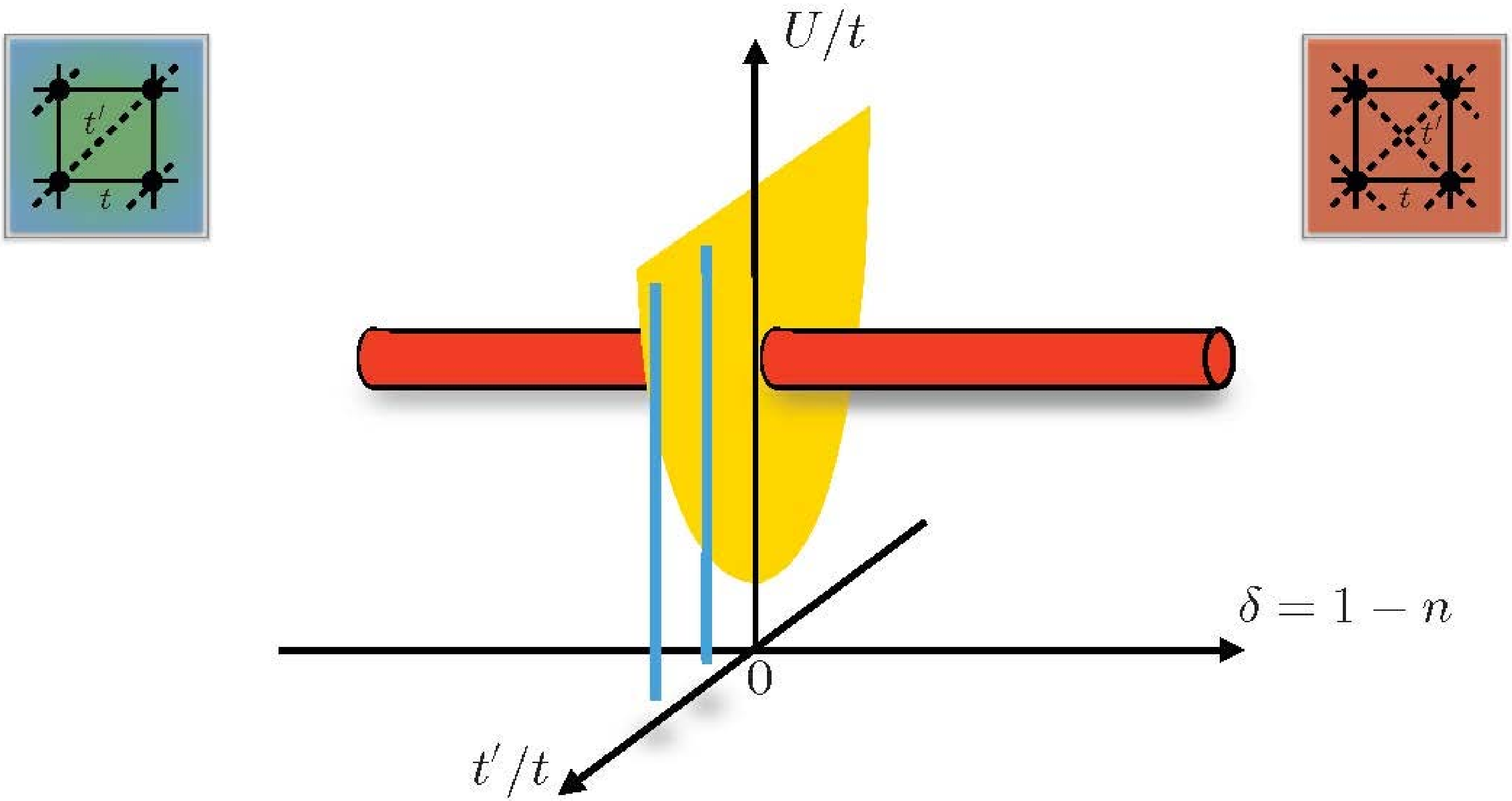
Perspective



Perspective



Perspective



Method

- Dynamical Mean Field Theory
  – clusters
- Concept: atomic-like localized correlations consistent with delocalized aspect

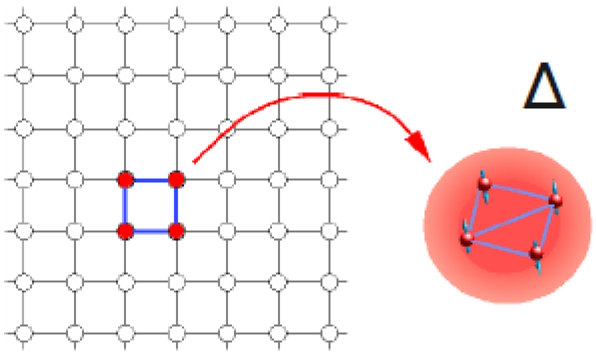
REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

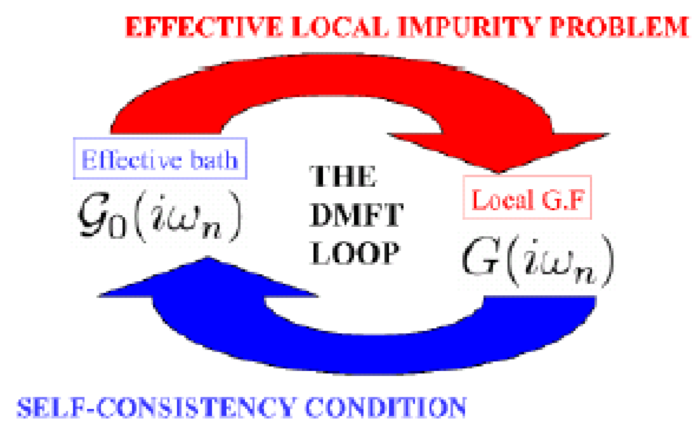
Hettler *et al*, PRB 1998
Lichtenstein *et al.*,PRB 2000
Kotliar *et al.*, PRB 2000
M. Potthoff, EJP 2003

Cellular DMFT + CT-QMC

E. Gull, A J. Millis, A. I. Lichtenstein, A. N. Rubtsov. M. Troyer. P. Werner, RMP **83**, 350 (2011)

$$Z = \int D[d^\dagger, d] \exp\left[-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i [d_i^\dagger(\tau) \Delta_{i'i}(\tau,\tau') d_{i'}(\tau')] \right]$$





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

-

+ and -

- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath (mean-field)
- Included exactly:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome, Kato, Kawasugi

Outline

- The model
- The method

- Part I: Half-filling (Mott insulator)
- Part II: Cuprates
  - Pseudogap
  - Strongly correlated superconductivity
- Part III: Organics
  - Half filling: insulator and superconductor
  - Doped case

Part I

Half-filling

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Giovanni Sordi

Lorenzo Fratino

Maxime Charlebois

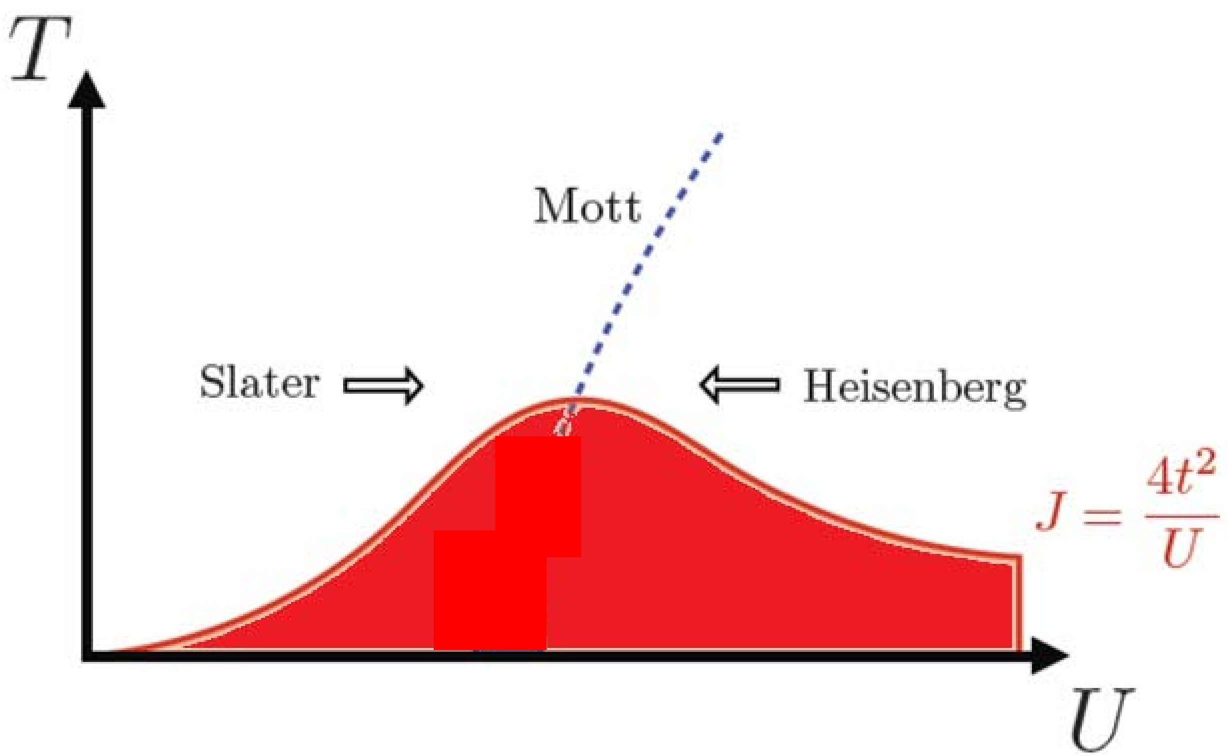
Patrick Sémon

Mott transition and antiferromagnetism

L. Fratino, P. Sémon, M. Charlebois, G. Sordi, AMT Phys. Rev. B **95**, 235109 (2017)

Underlying Mott transition

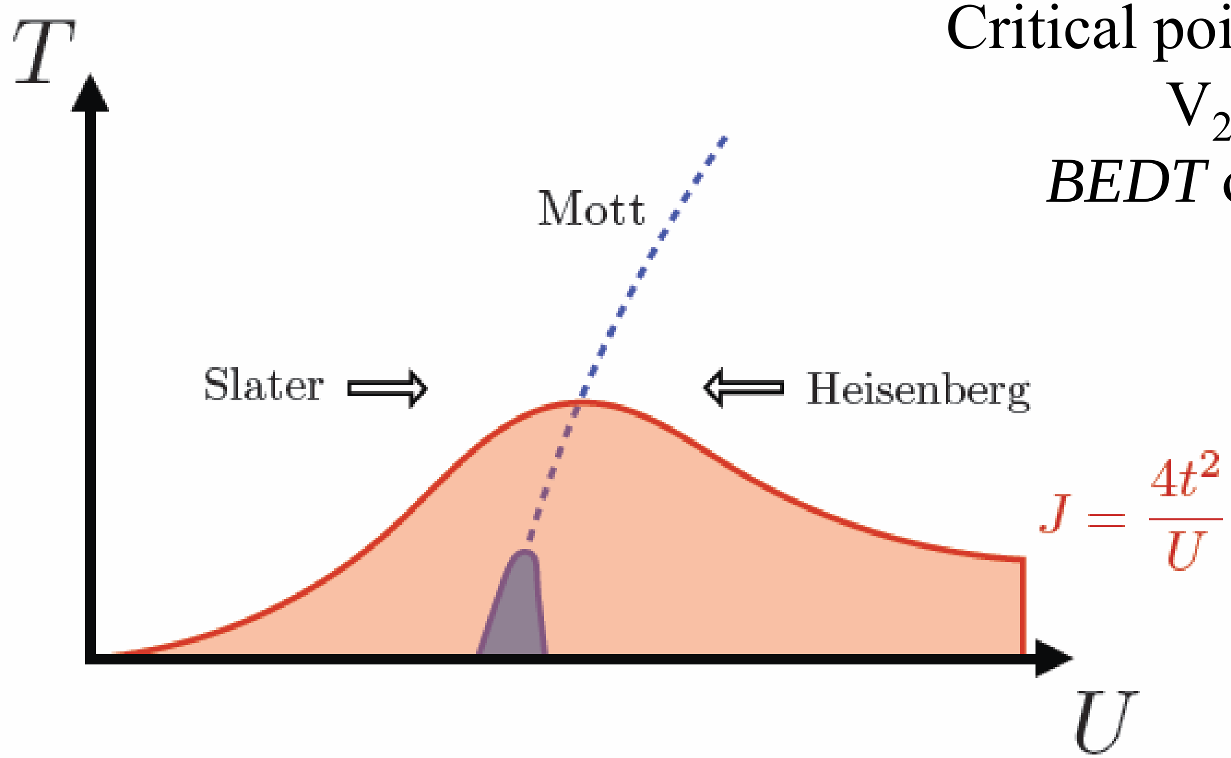
n = 1, d = 3



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

Underlying Mott transition

n = *1*, *d* = *3*



Critical point visible in V_2O_3, *BEDT* organics

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

Part II: Cuprates

- Pseudogap

Giovanni Sordi

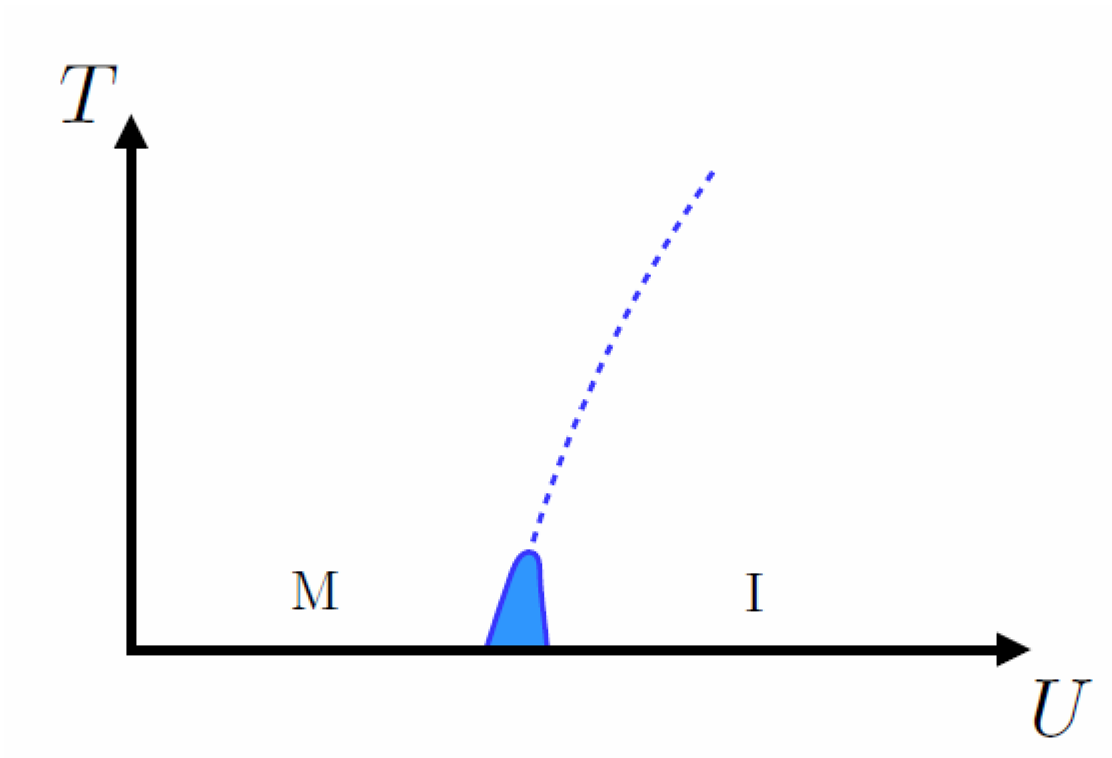
Kristjan Haule

Pseudogap from the influence of the Mott transition away from half-filling

Sordi et al., PRL 104, 226402 (2010)
Sordi et al., PRB 84, 075161 (2011)
Fratino et al., PRB 93, 245147 (2016) [Emery model]
Sordi et al., Sci. Rep. 2 547 (2012);
Sordi et al., PRB 87, 041101(R) (2013)
Fratino et al., PRB 93, 245147 (2016) [Emery model]

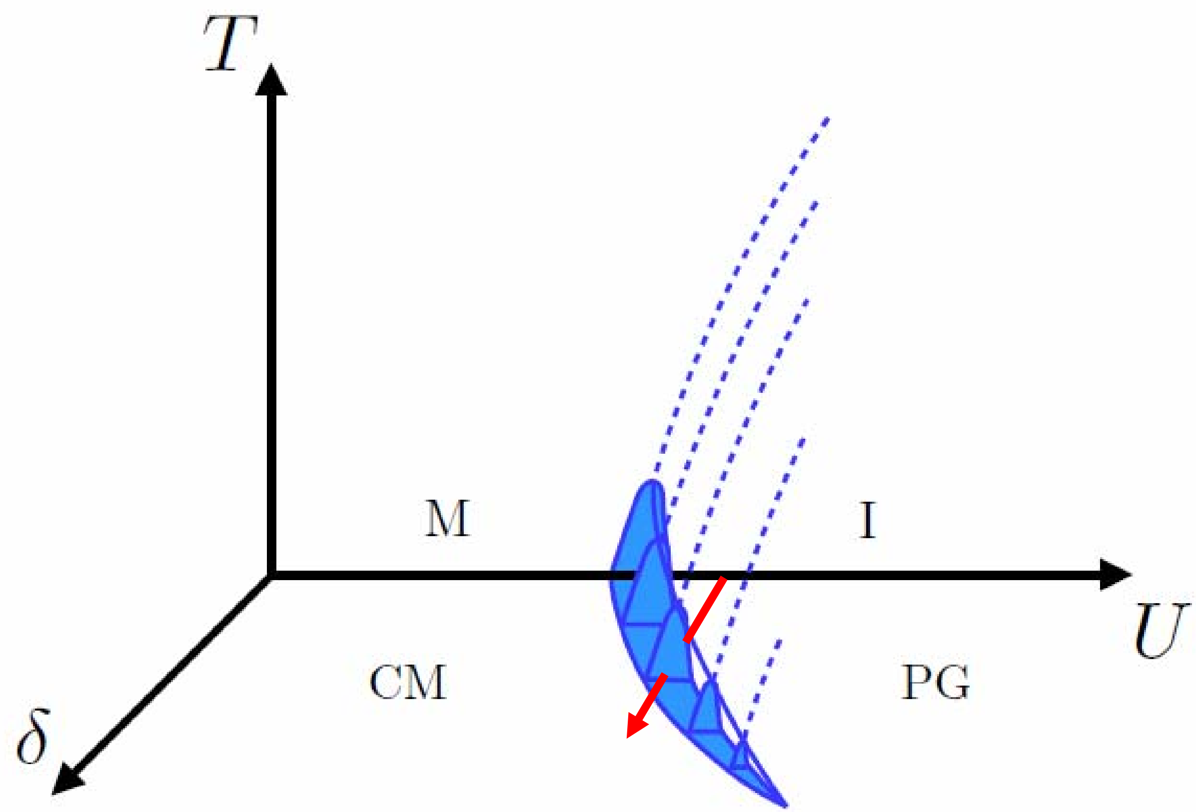
Influence of Mott transition away from half-filling

$n = 1$, $d = 2$ square lattice



Influence of Mott transition away from half-filling

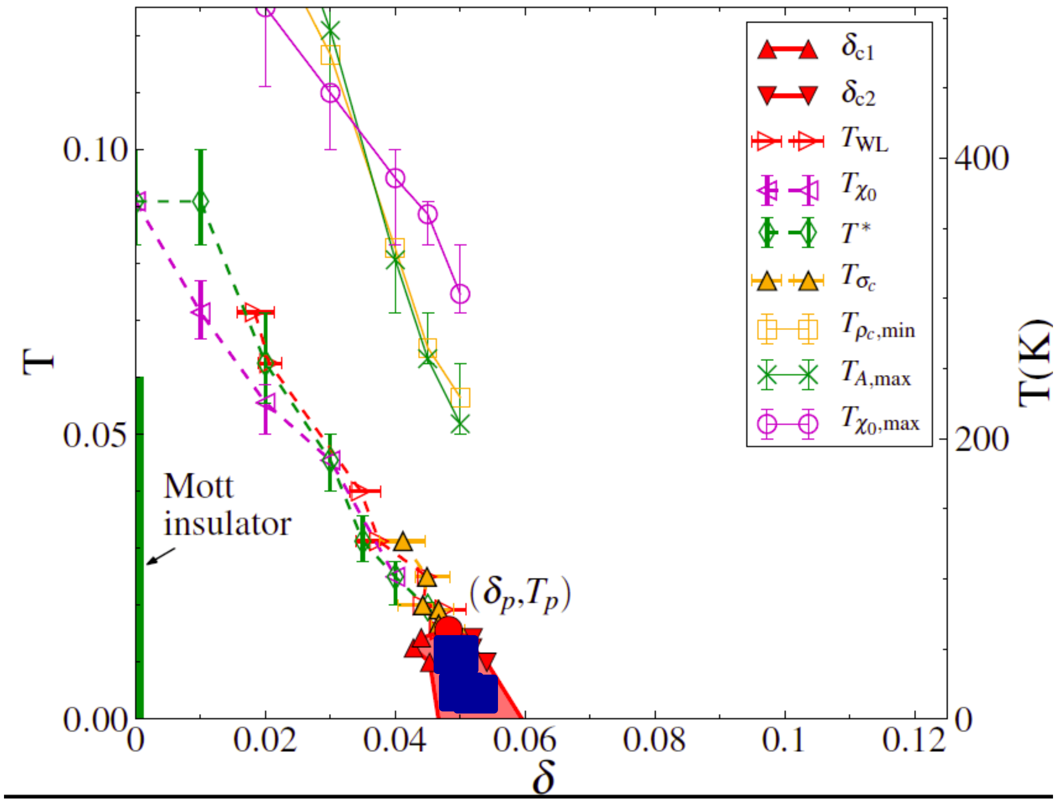
$n = 1$, $d = 2$ square lattice



Two crossover lines

Widom line

Giovanni Sordi

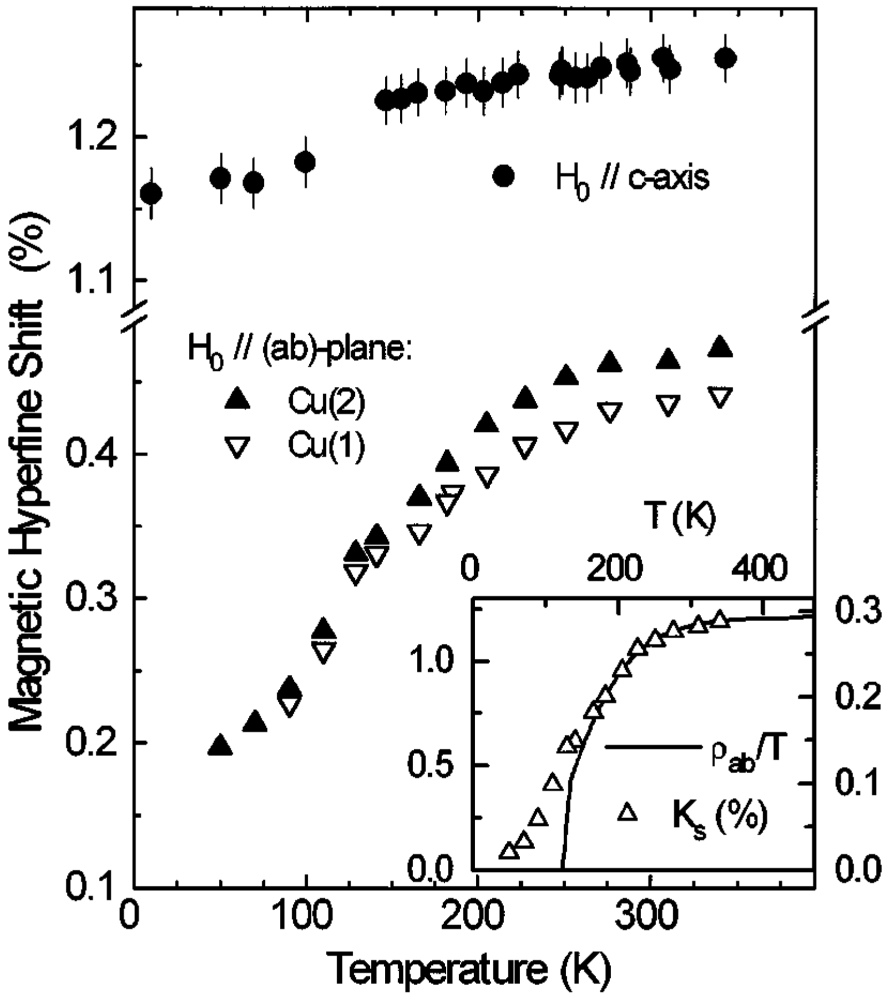


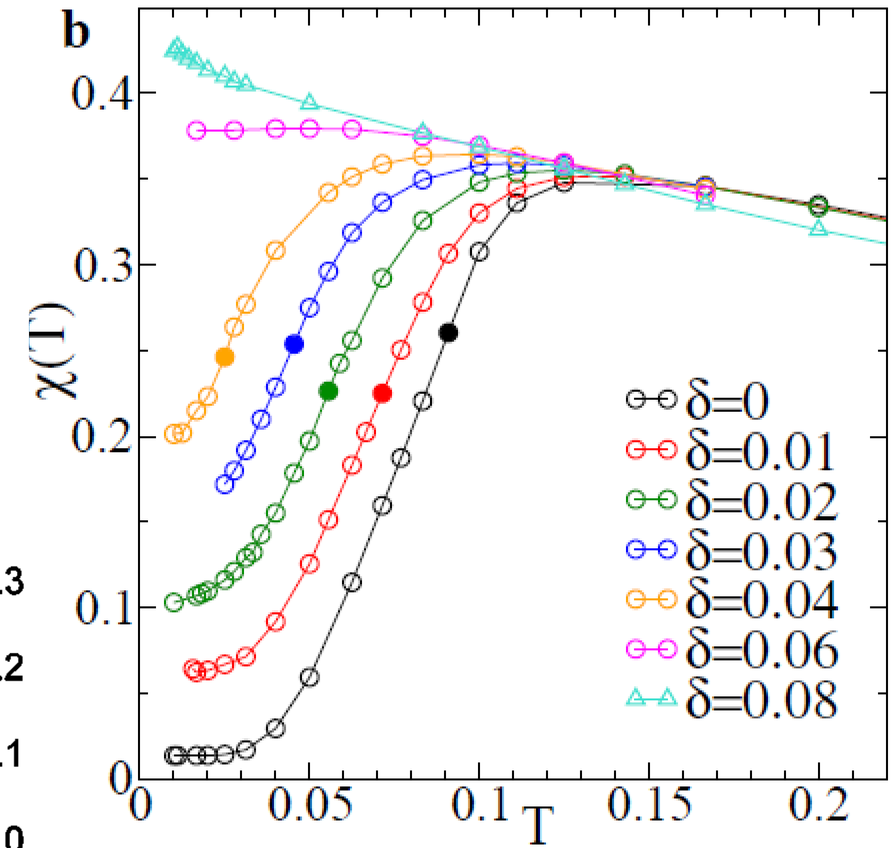
Patrick Sémon

G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

Spin susceptibility

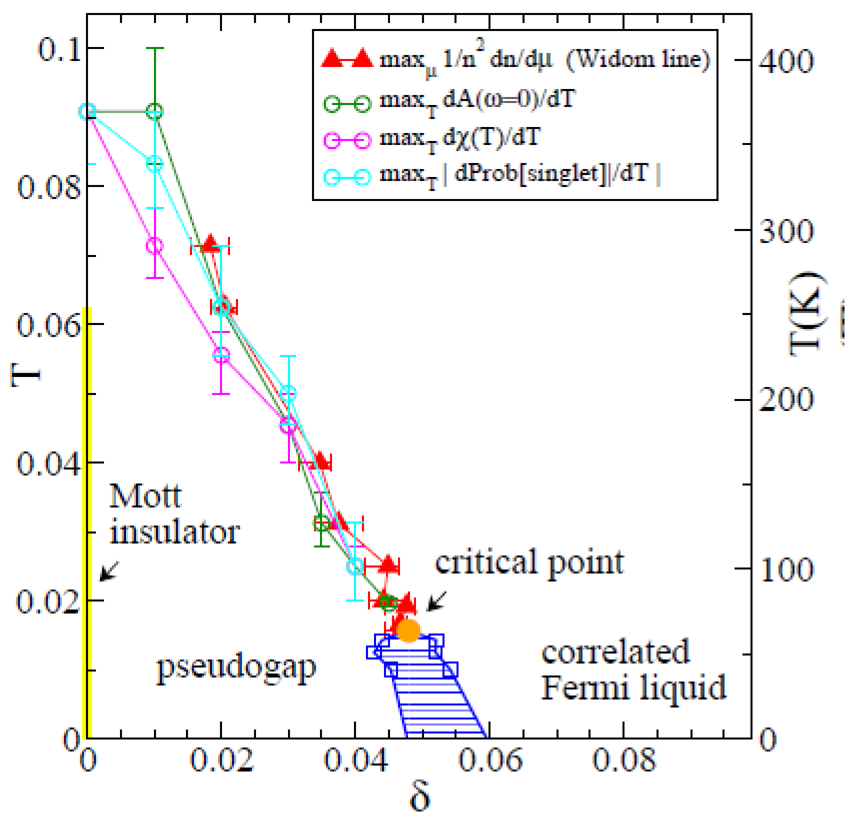


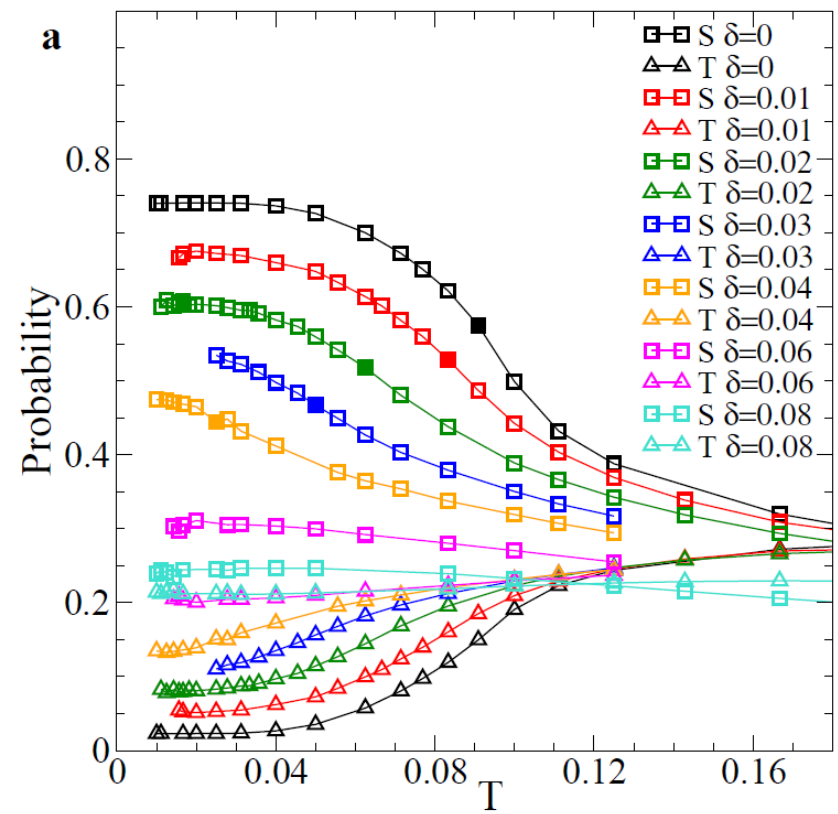


Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
PRB **80**, 064501 (2009)

Part II: Cuprates

- Strongly correlated superconductivity

Giovanni Sordi

Patrick Sémon

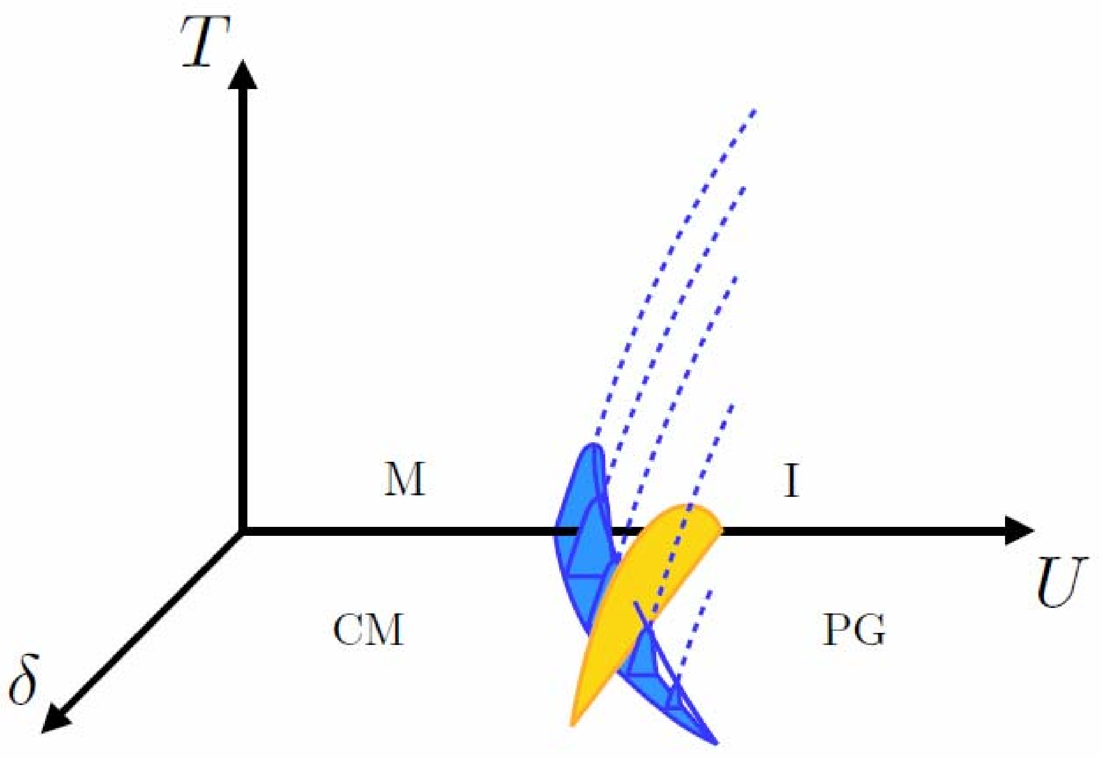
Lorenzo Fratino

Superconductivity in a doped Mott insulator

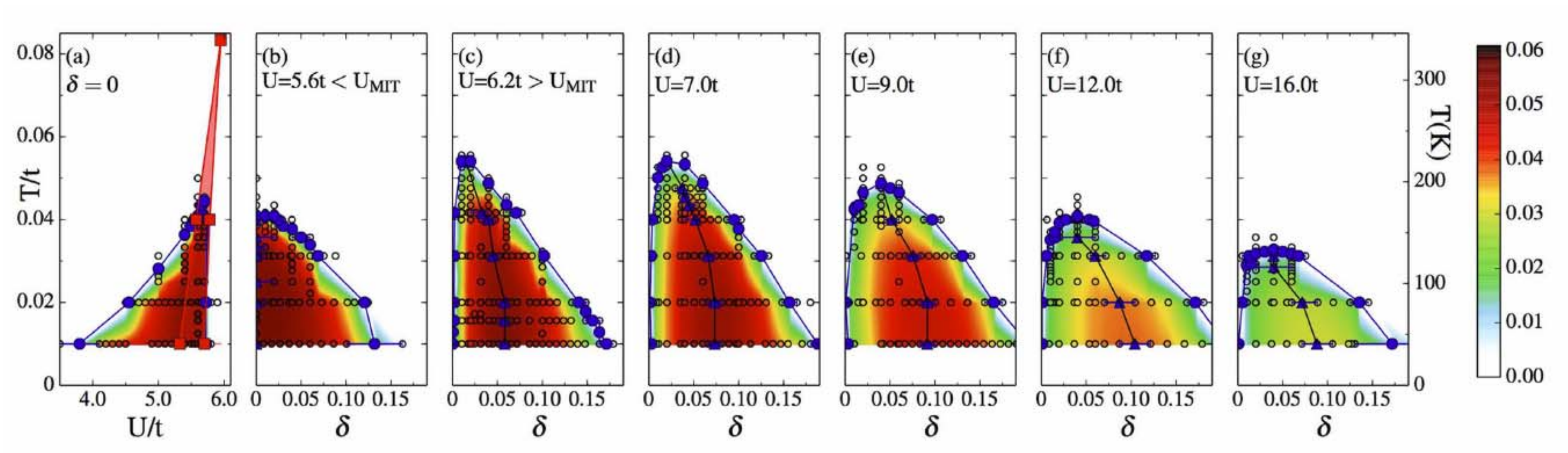
Sordi et al. PRL **108**, 216401 (2012)
Fratino et al.
Sci. Rep. **6**, 22715 (2016)

Superconductiviy in Doped Mott insulator

$n = 1, d = 2$ square lattice



T_c controlled by J



Fratino et al.
Sci. Rep. **6**, 22715

Some experiments that suggest $T_c < T_{pair} < T^*$

T. Kondo *et al*. PRL **111** (2013)

Kondo, Takeshi, et al. Kaminski Nature Physics 2011, *7*, 21-25

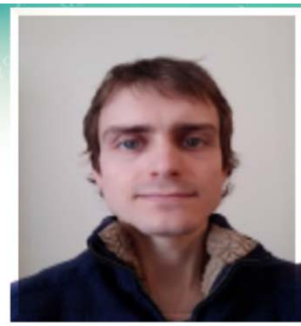
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)


Olivier Simard


Charles-David Hébert


Alexandre Foley

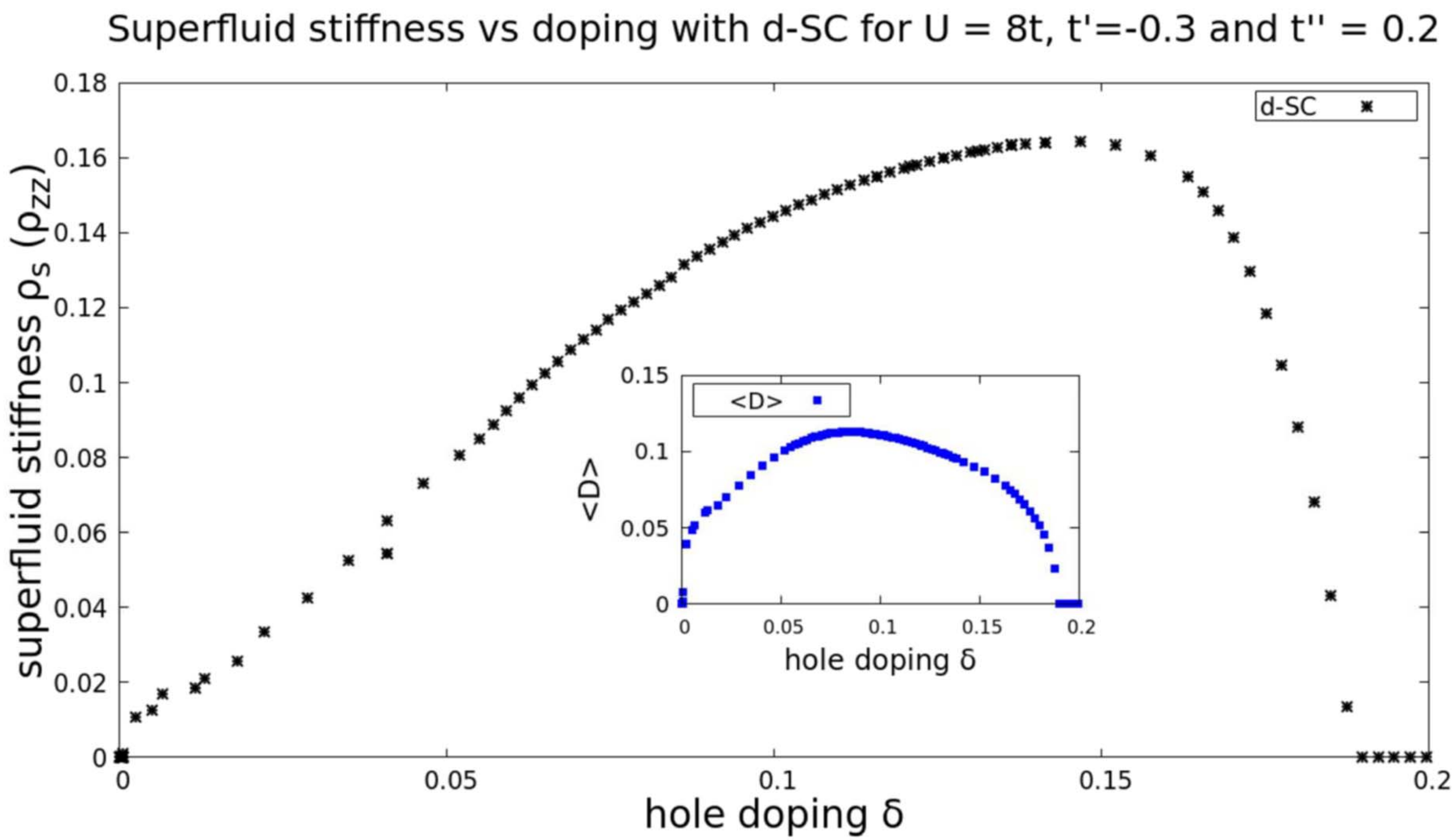

David Sénéchal

What causes T_c to drop near $n = 1$?

O. Simard, C.-D. Hébert, A. Foley, A.-M.S. Tremblay, D. Sénéchal, unpublished

Superfluid stiffness *T=0*

$$\rho_{ab} = \langle \hat{J}_a(\boldsymbol{r},\tau)\,\hat{J}_b(\boldsymbol{r}',\tau')\rangle = \frac{-\beta}{V}\frac{\delta^2\mathcal{F}}{\delta A_a(\boldsymbol{r},\tau)\,\delta A_b(\boldsymbol{r}',\tau')}\bigg|_{\boldsymbol{A}=0}$$



Part III: Organics

- Half-filling: insulator and superconductor

Charles-David Hébert

Patrick Sémon

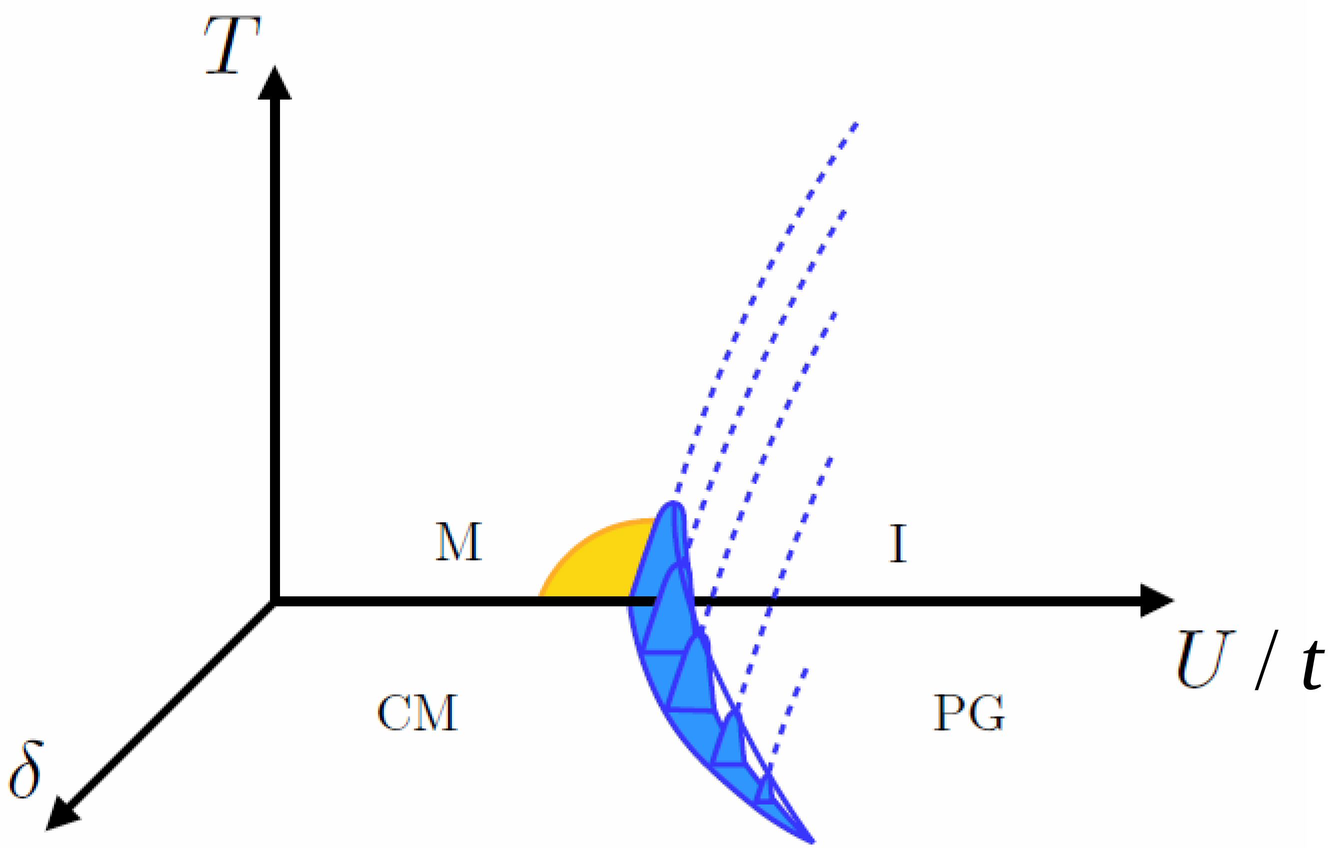
Organics : Phase diagram, finite T

Made possible by algorithmic improvements

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

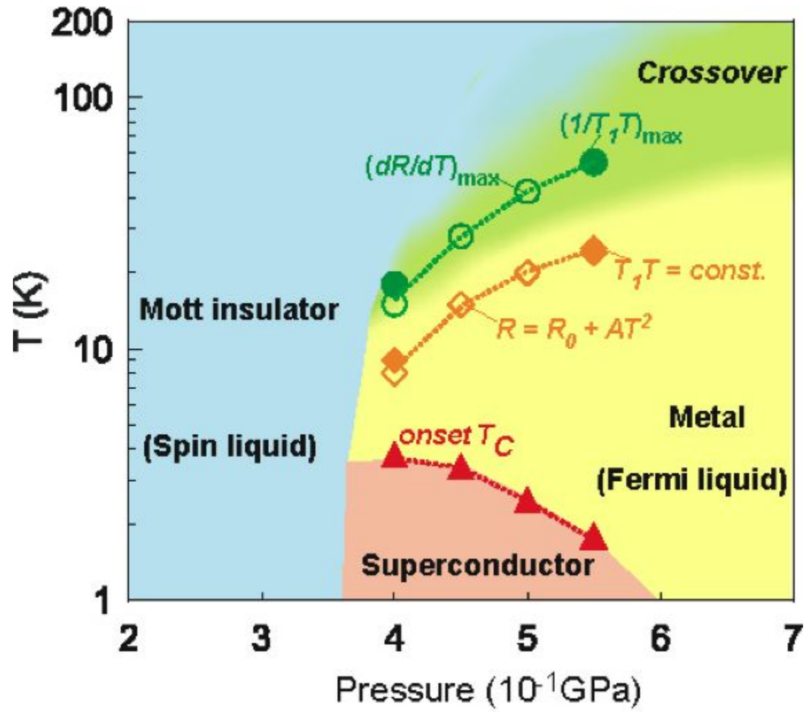
Superconductivity near the Mott transition

n = 1, d = 2 square lattice



Phase diagram at *n = 1*

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

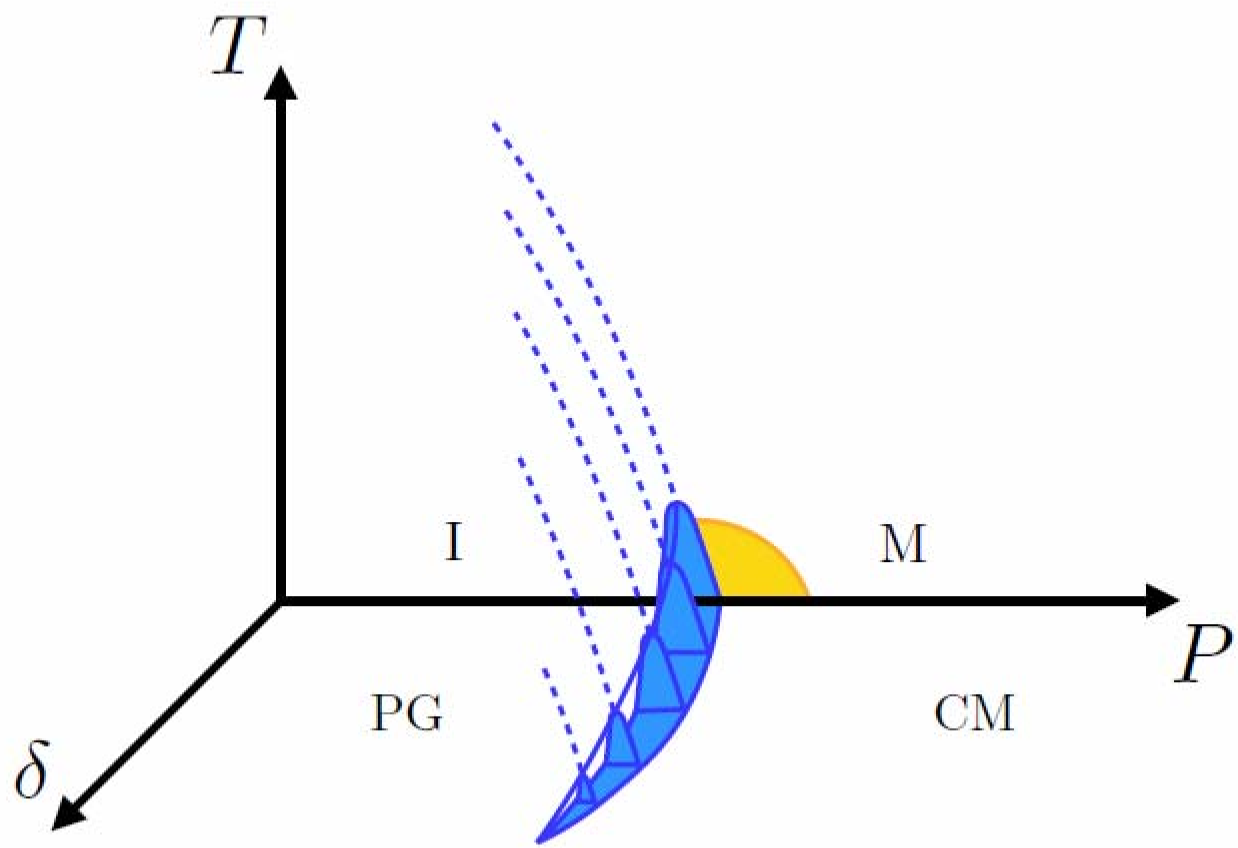


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

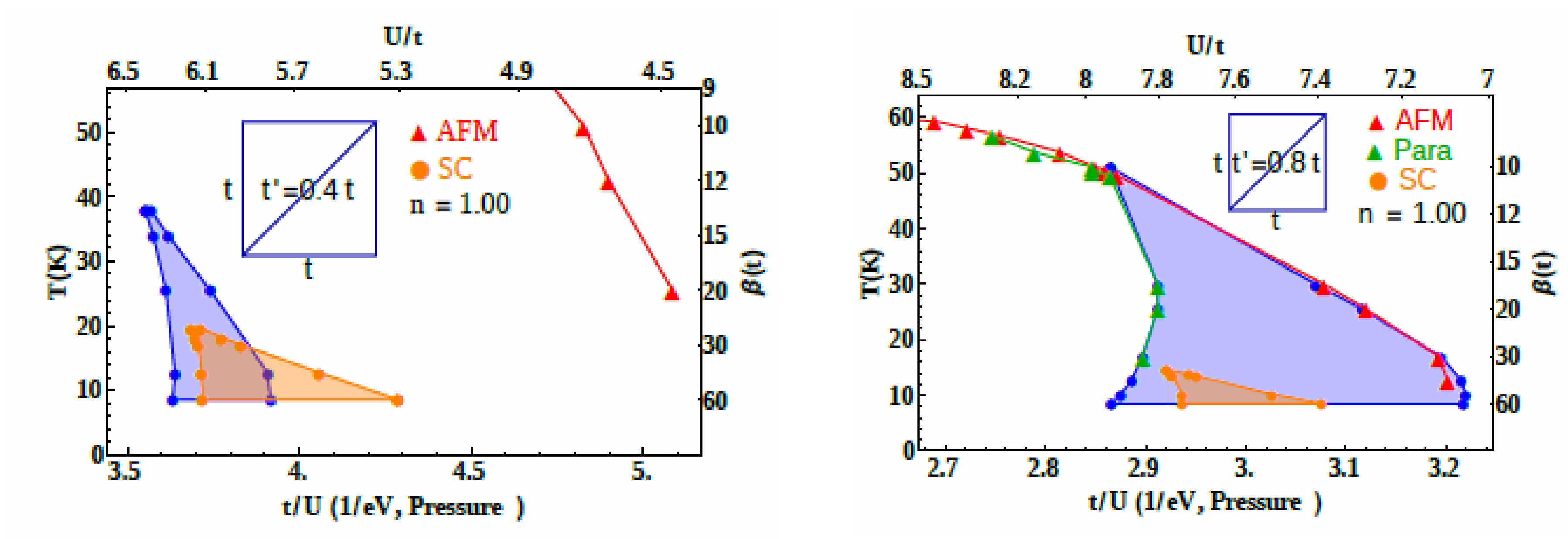
Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

Superconductivity near the Mott transition

$n = 1$, $d = 2$ square lattice



Superconductivity near Mott transition (*n = 1*)



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

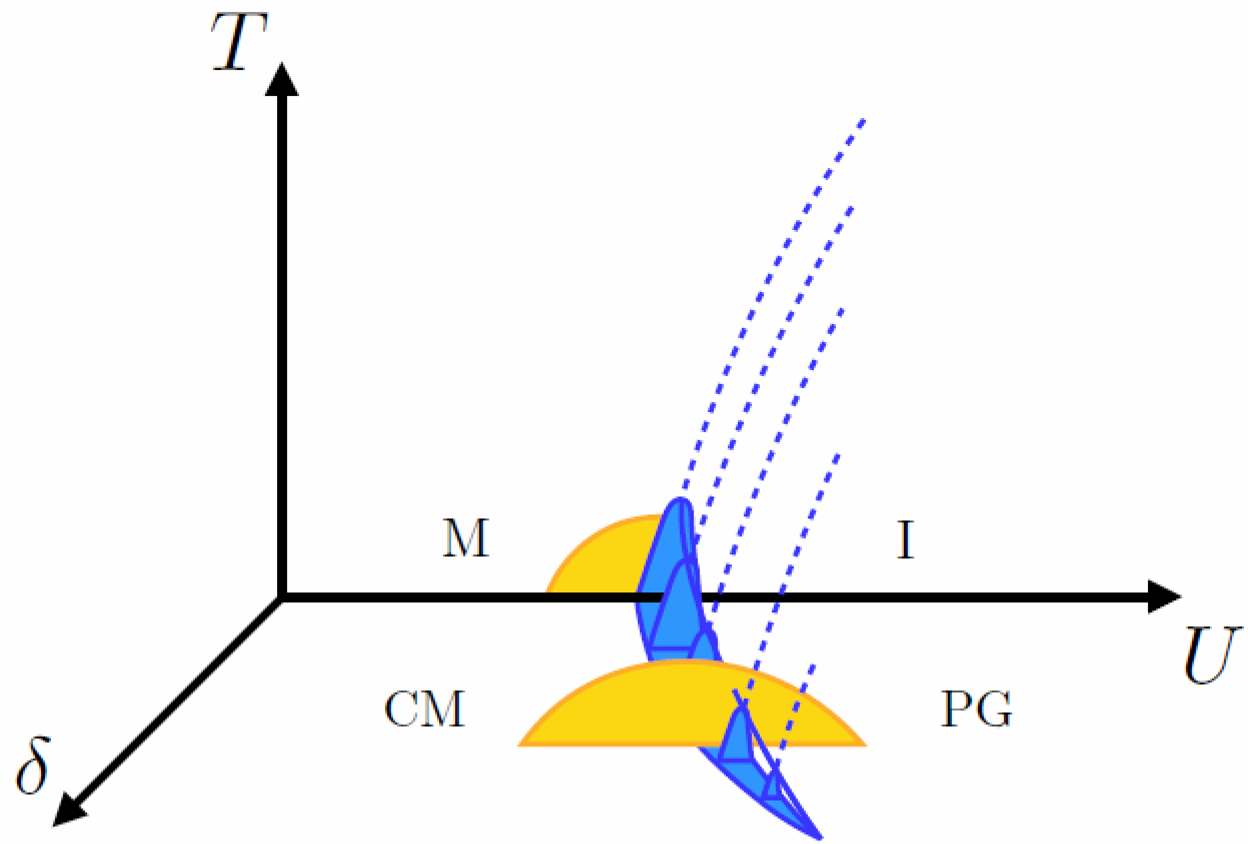
Part III: Organics

- Doped case

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

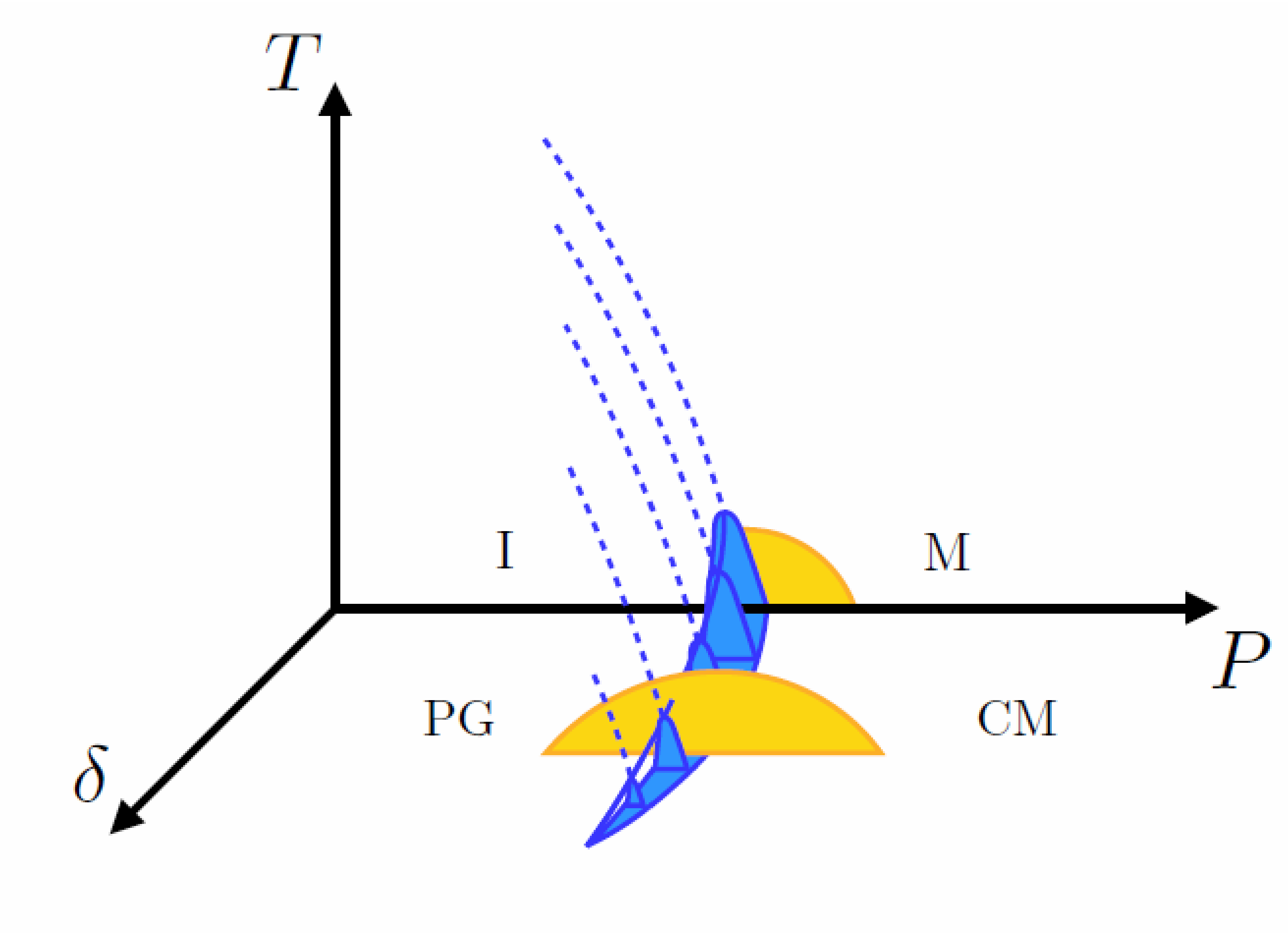
Doped organics

n = 1, d = 2 square lattice

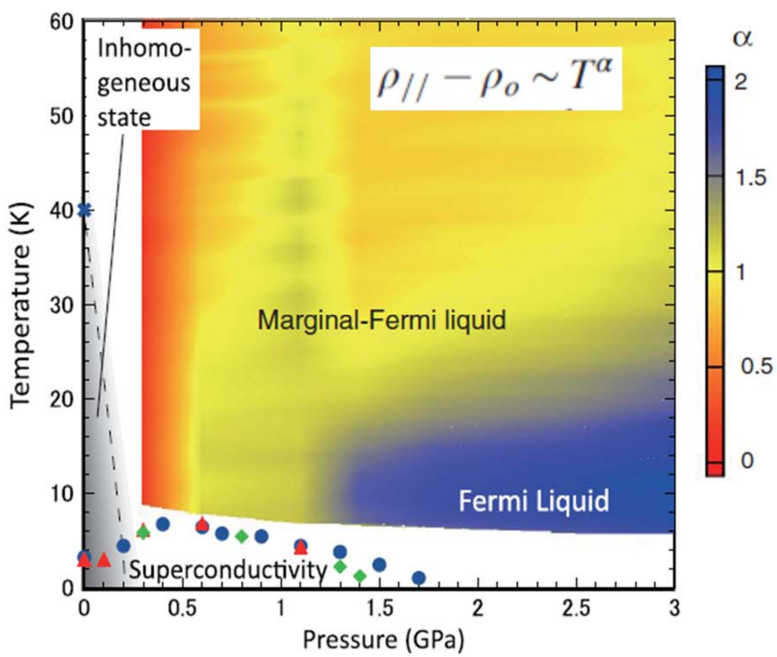


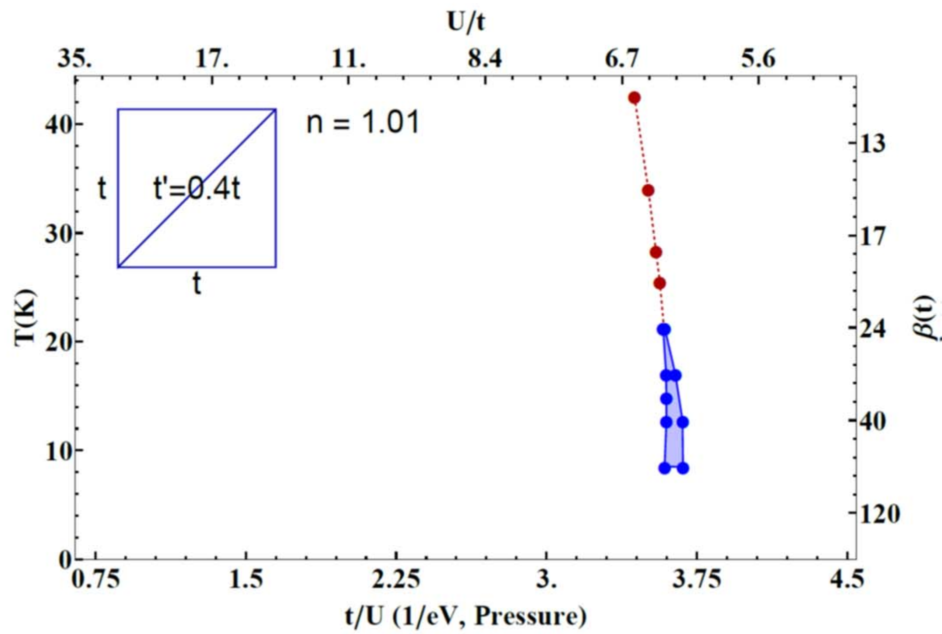
Doped organics

$n = 1$, $d = 2$ square lattice



Doped organics: Crossover

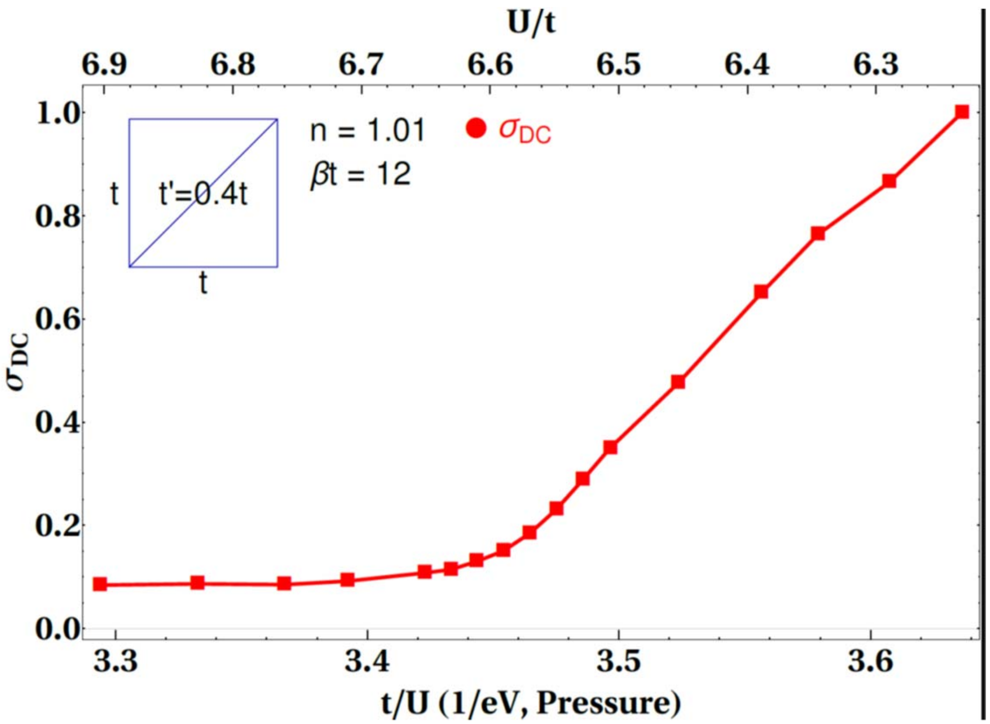


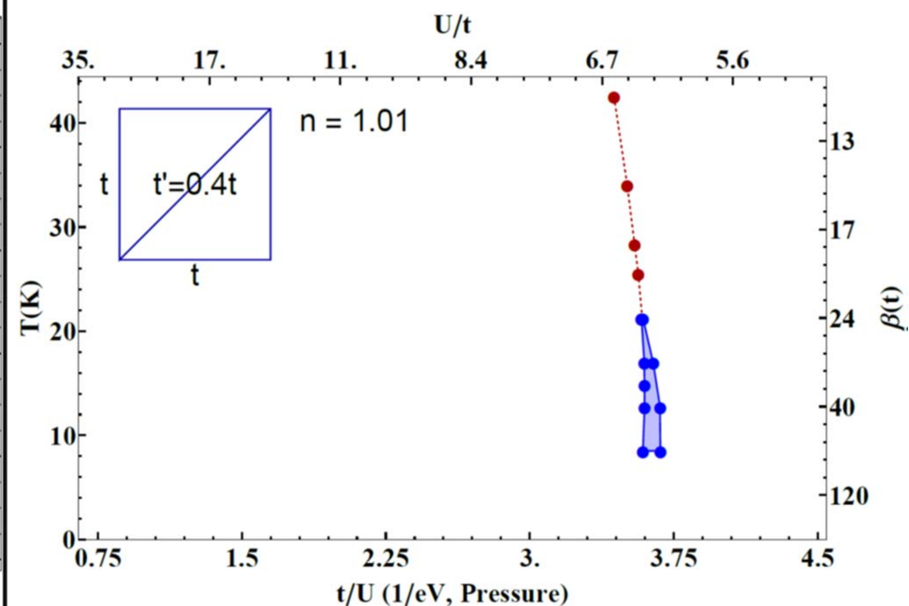


H. Oike, and al.
Phys. Rev. Lett. **114**,
067002(2015)

Charles-David Hébert, AMST, unpublished

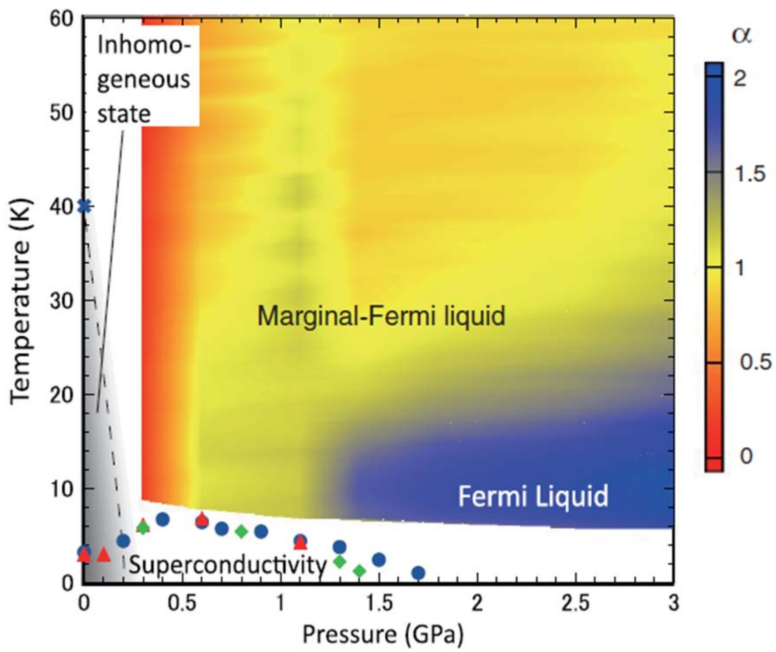
Doped organics: crossover



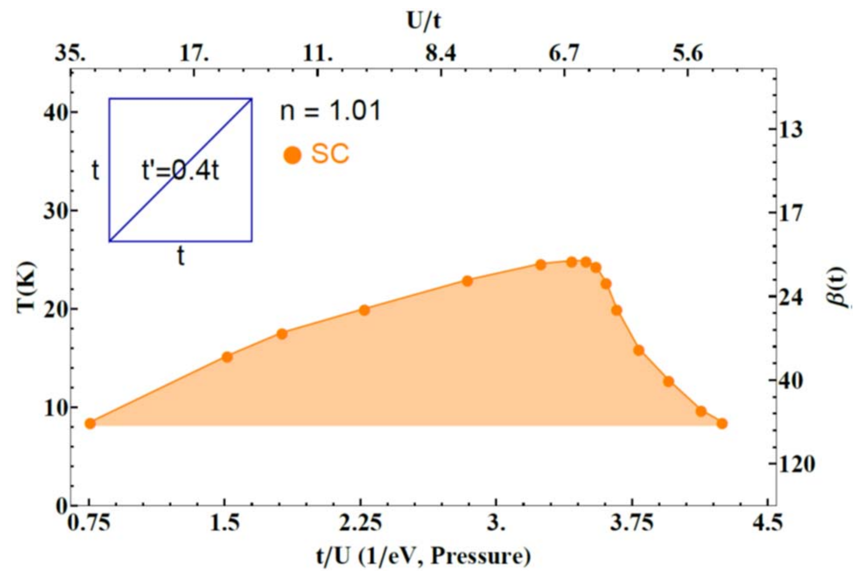


Charles-David Hébert, AMST, unpublished

Doped organics: superconductivity



H Oike, and al.
Phys. Rev. Lett. **114**, 067002(2015)

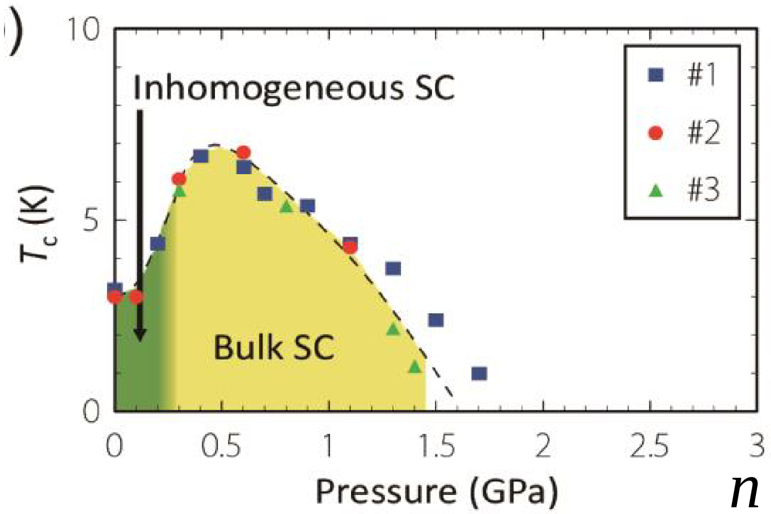


Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc.
3, 013004 (2014)

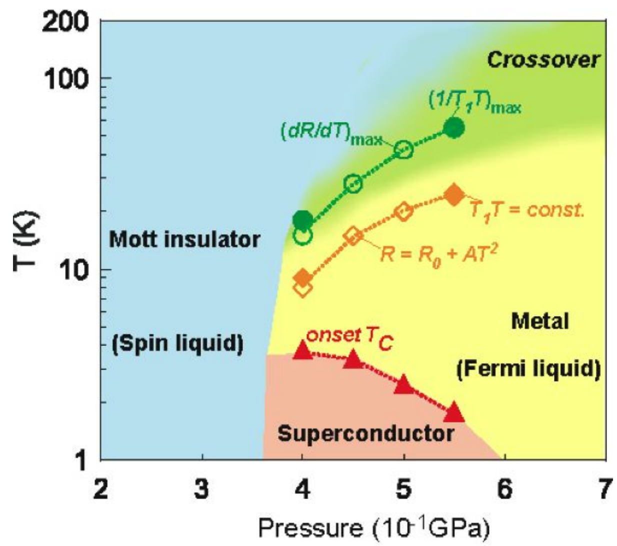
C.-D. Hébert, P. Sémon, A.-M.S. T PRB **92**, 195112 (2015)

Doped organics: superconductivity

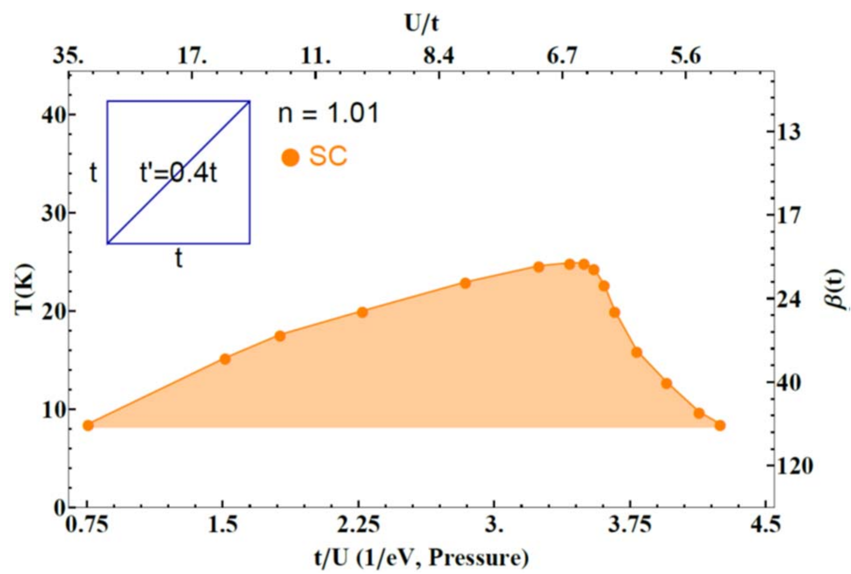
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)



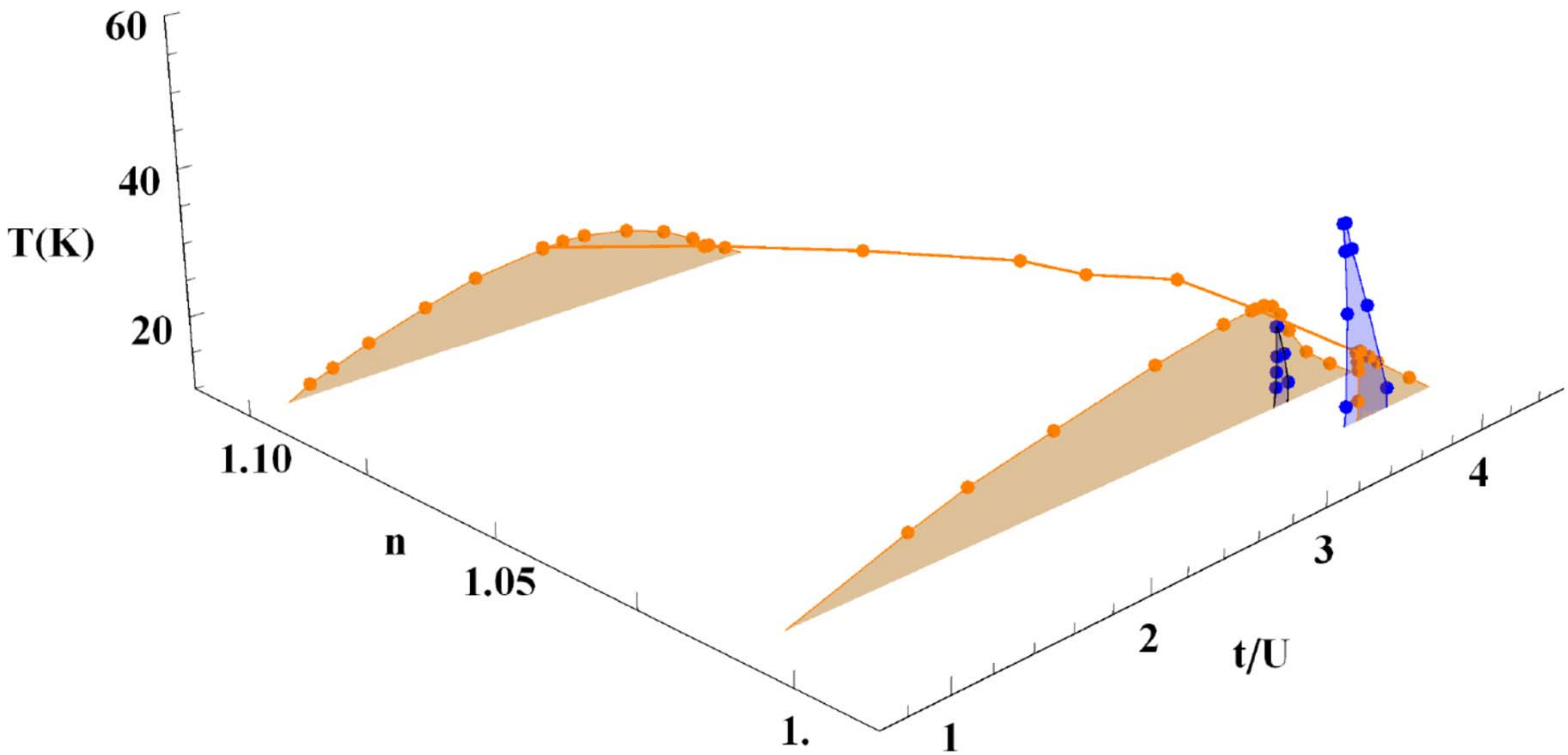
n = 0.90



n= 1

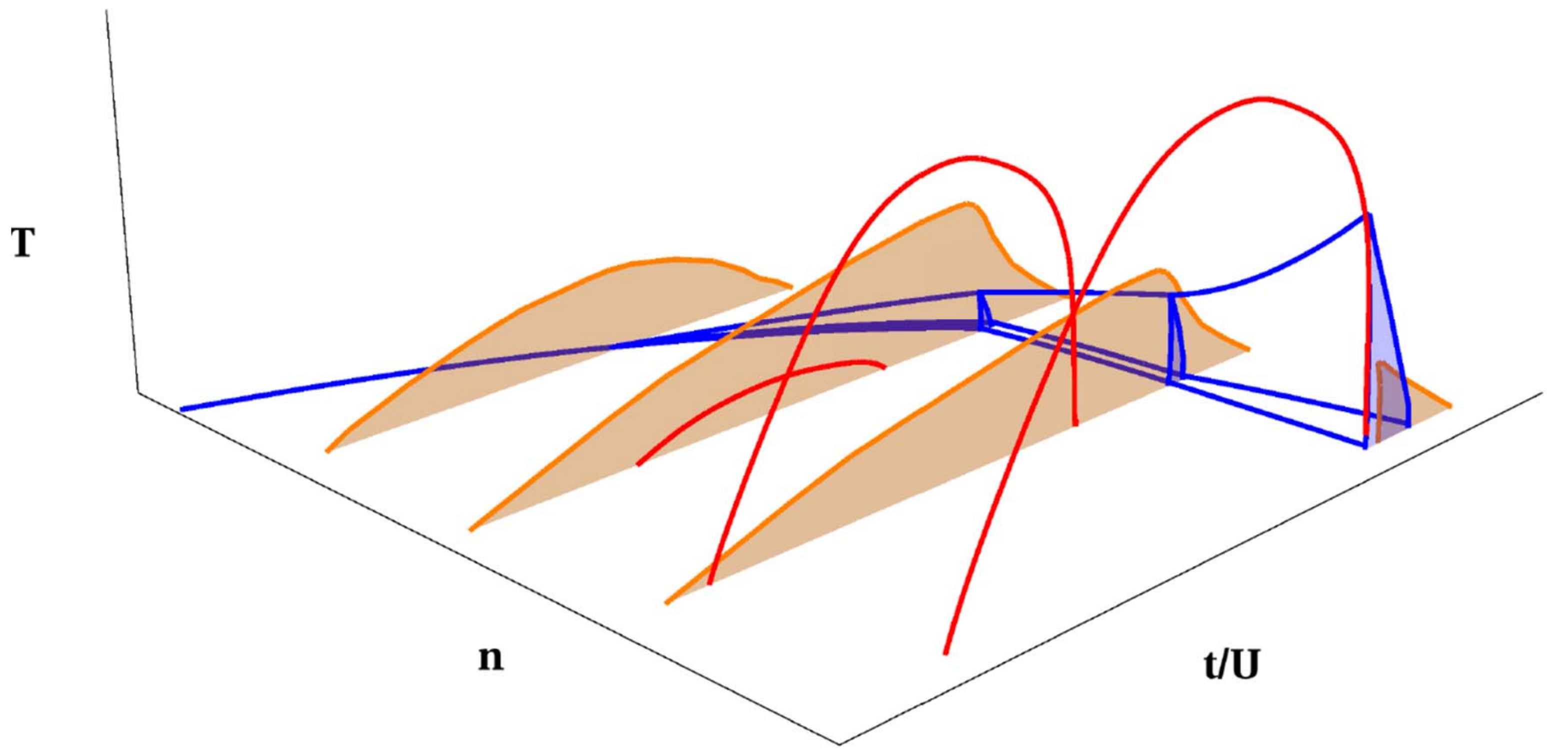


Doped organics: Overall phase diagram



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

Doped organics:
Schematic phase diagram, strong frustration



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

Non BCS superconductivity

Charles-David Hébert, AMST, unpublished

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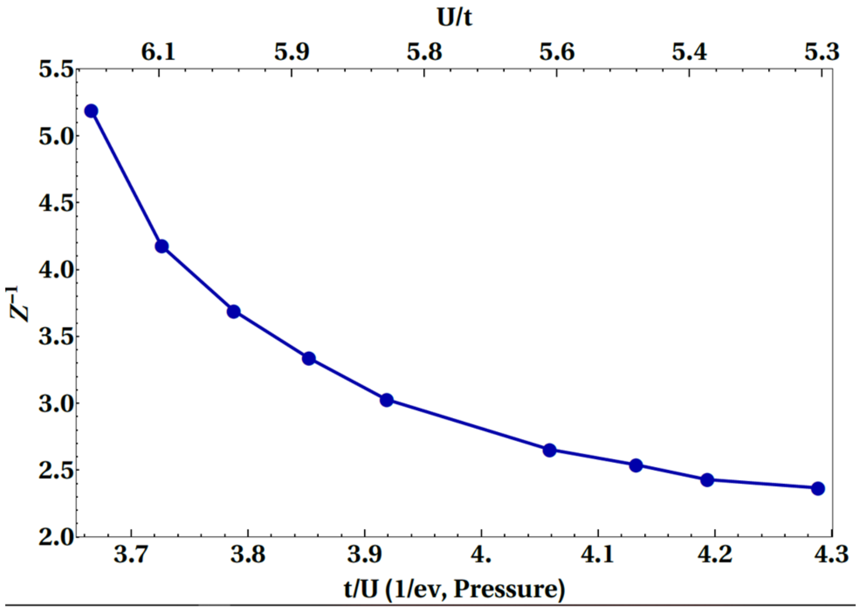
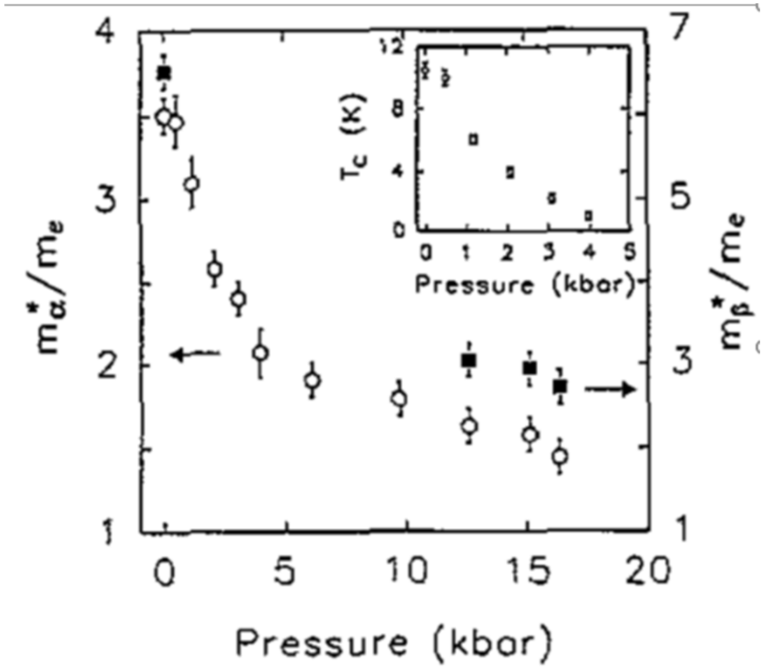
Superfluid stiffness: Effective mass

$$\rho_s = \frac{n_s e^2}{m^*}$$

M. I. Larkin and al. Phys. Rev. B 64, 144514 (2001)

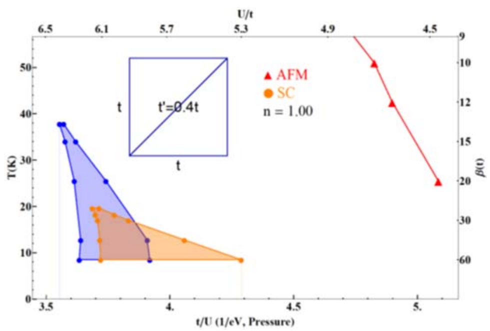
$\kappa - ET_2Cu[(NCS)_2]$

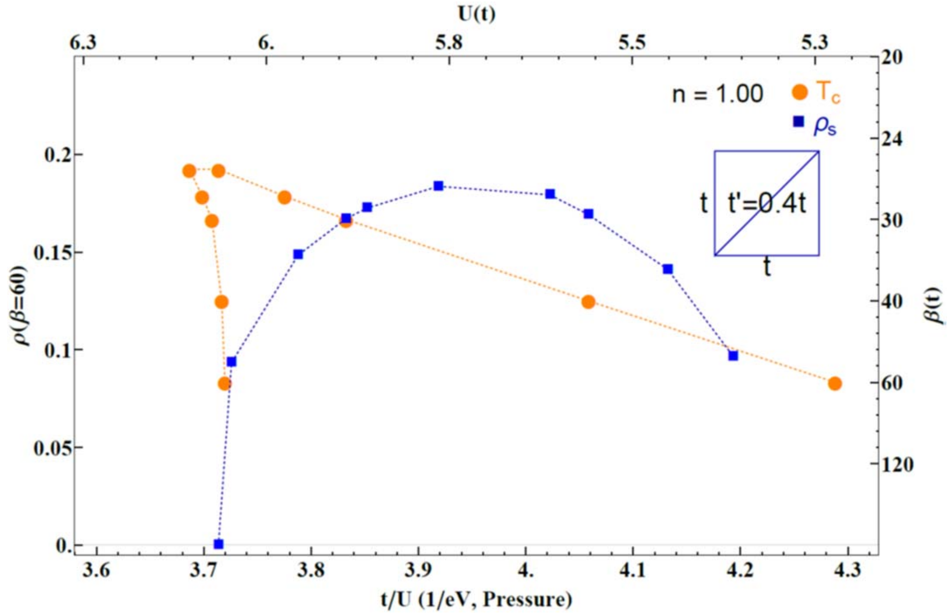




Superfluid stiffness: unusual

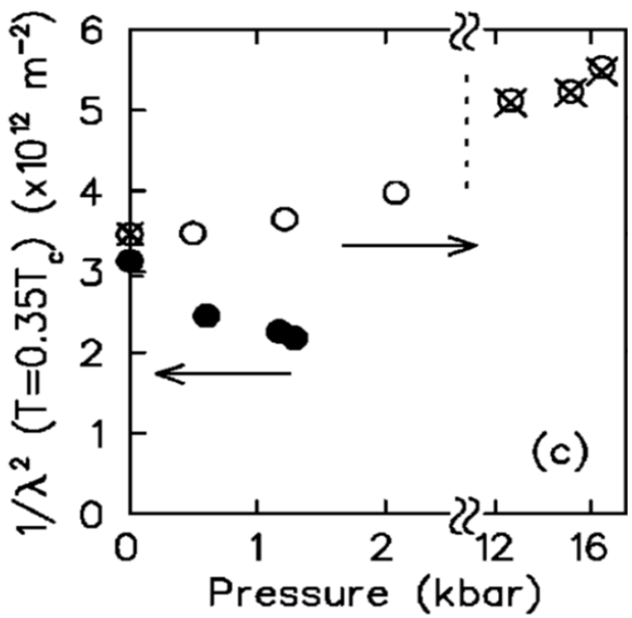
$$\rho_s = \frac{n_s e^2}{m^*} = \frac{1}{\lambda^2 \mu_0}$$



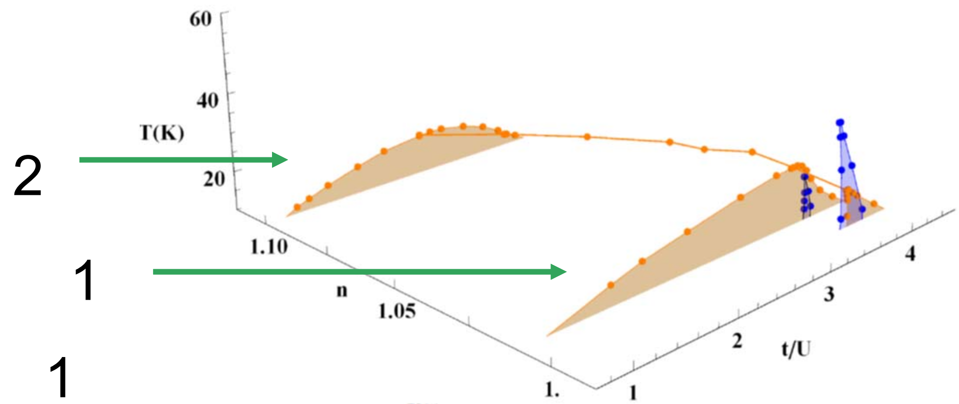


M. I. Larkin and al. Phys. Rev. B 64, 144514 (2001)

$\kappa - ET_2Cu[(NCS)_2]$



Superfluid stiffness



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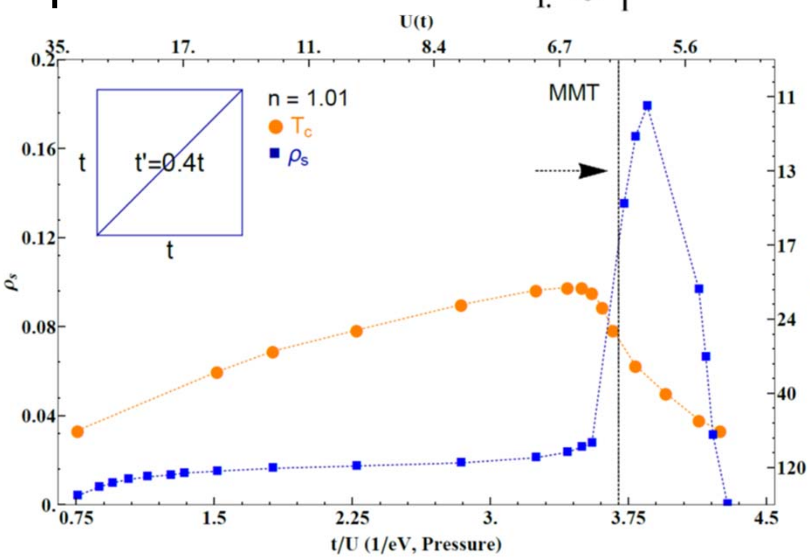

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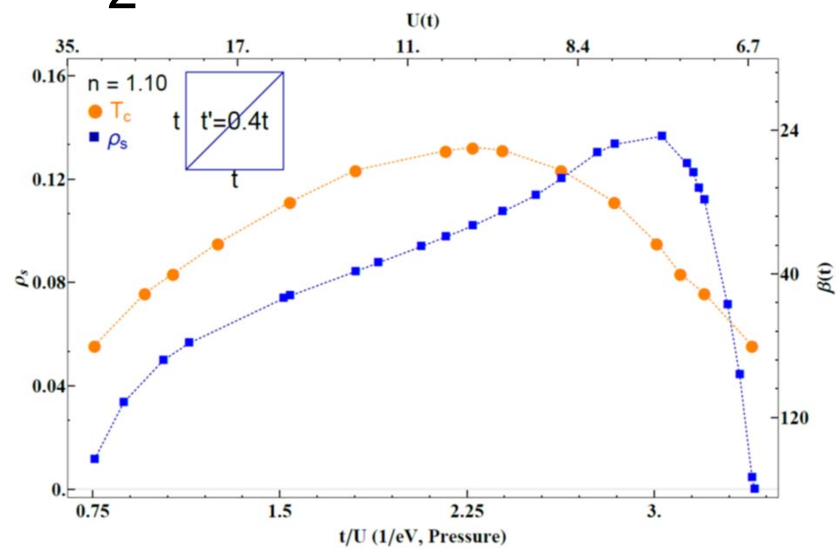

Summary

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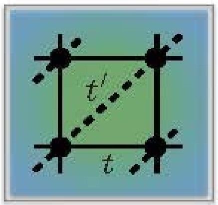
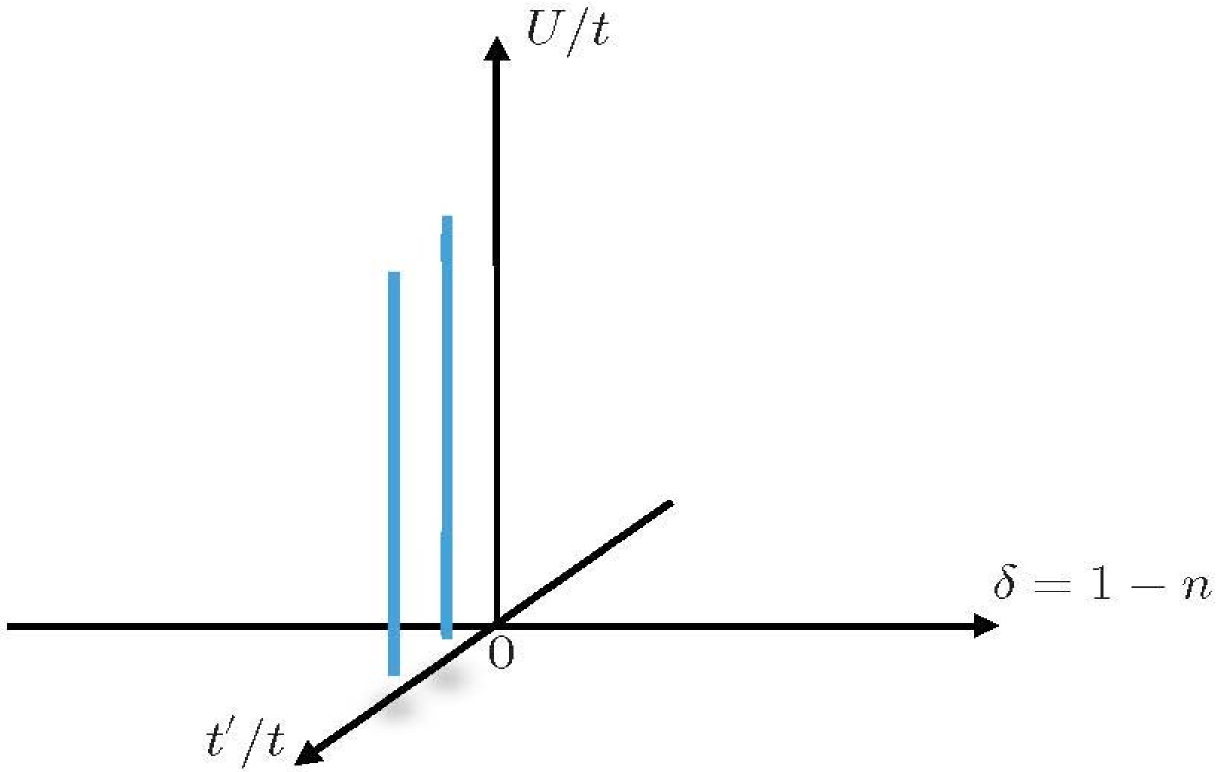
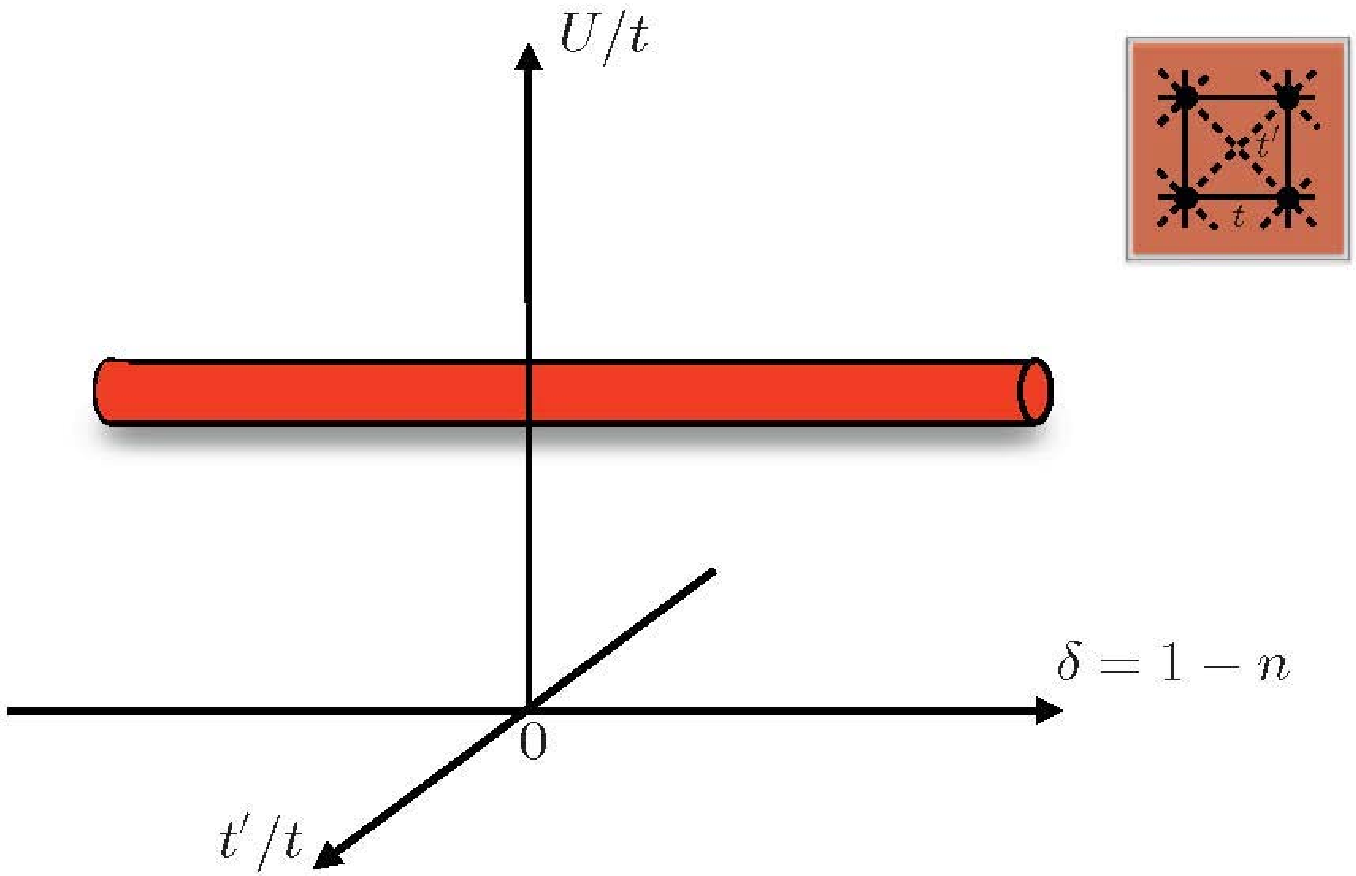
Perspective

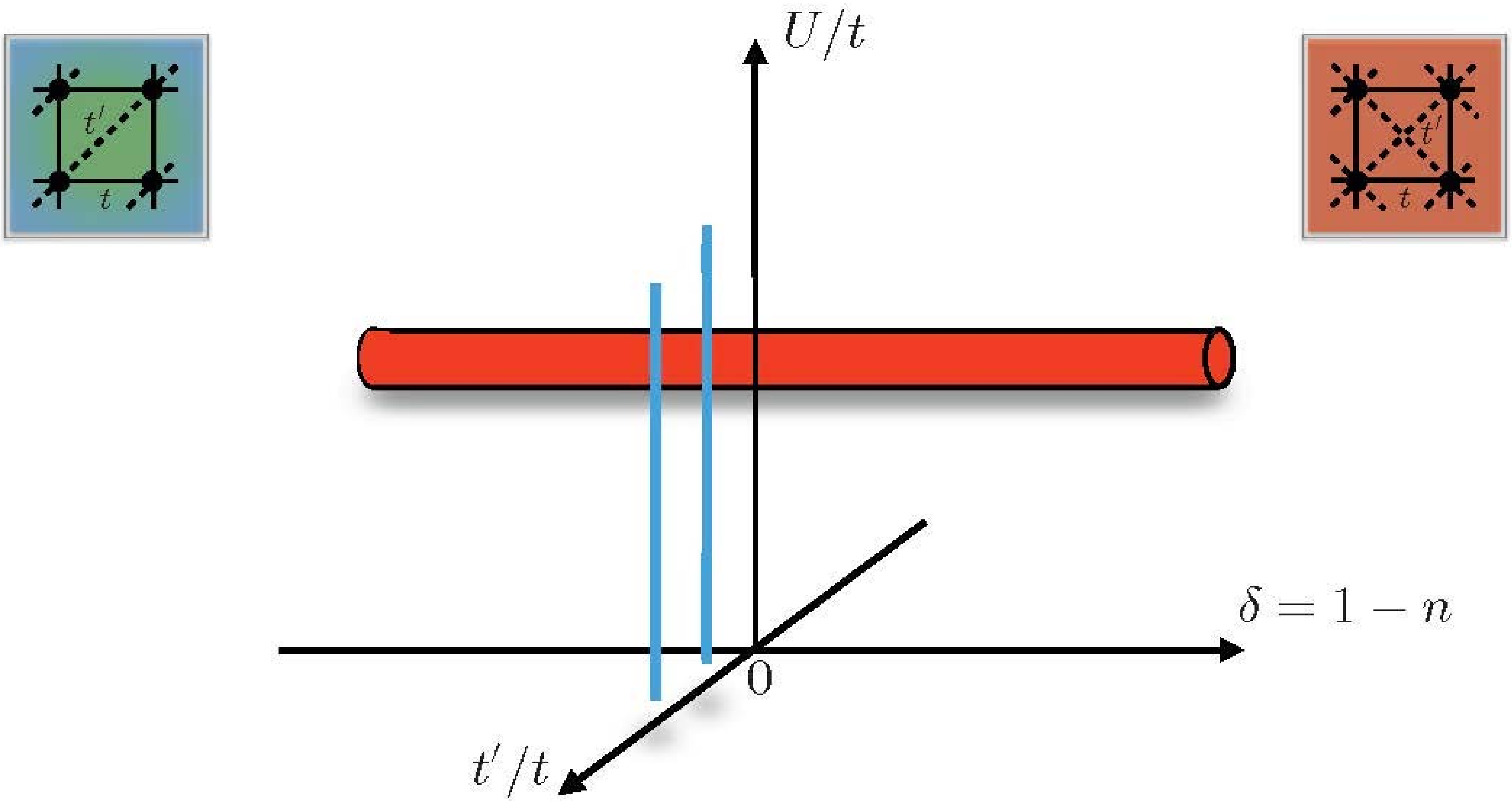




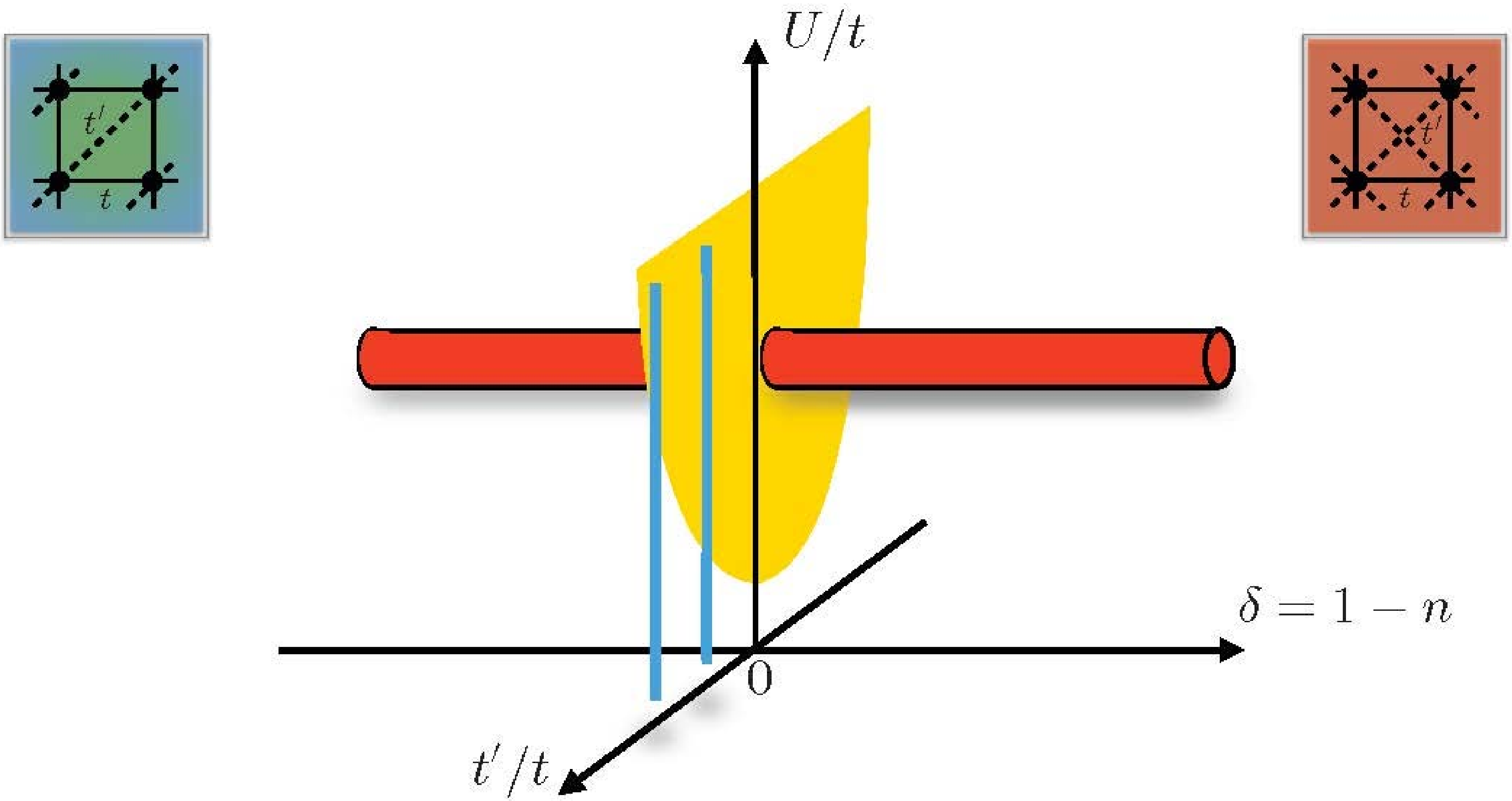
Perspective



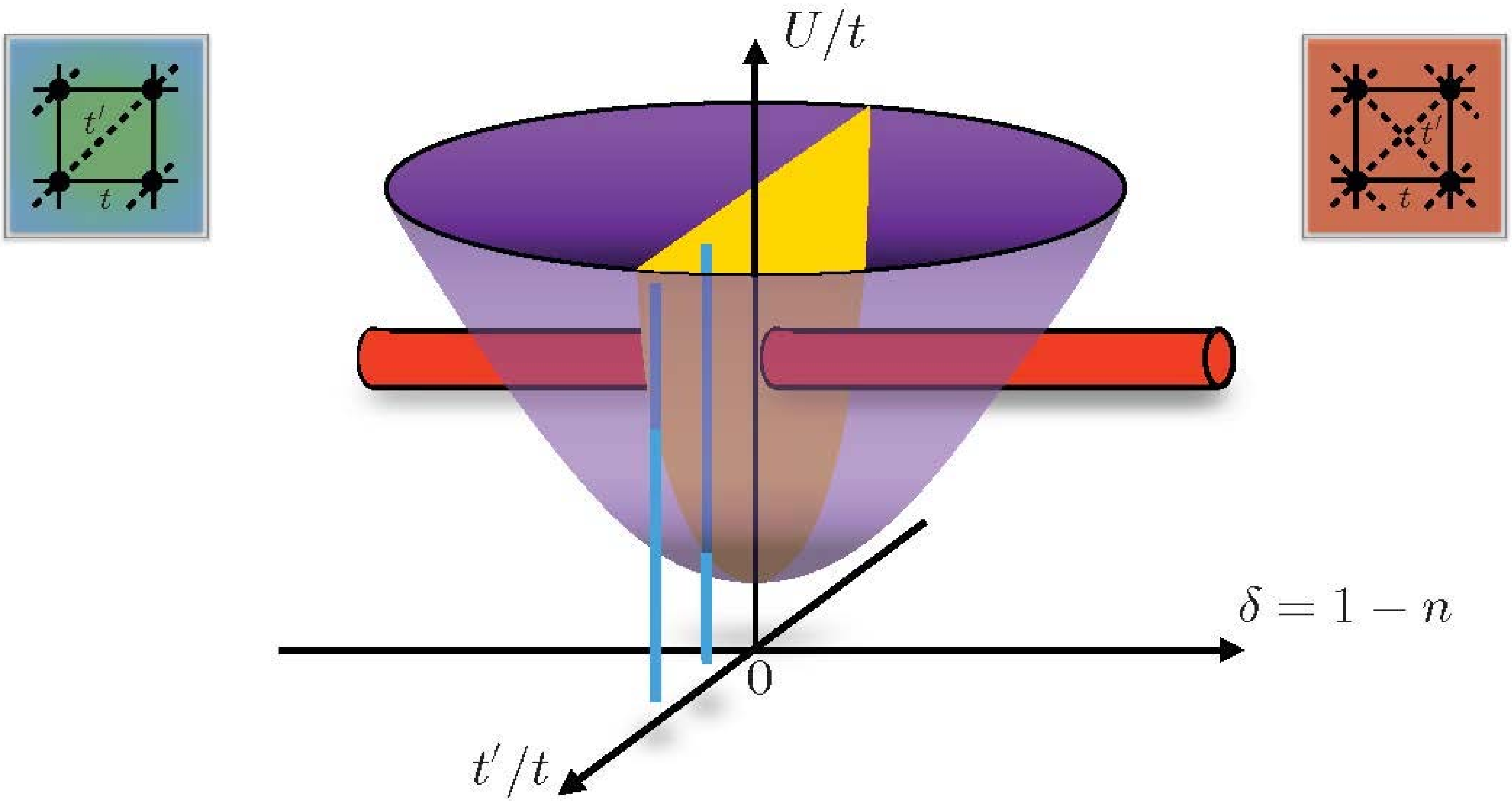
Perspective



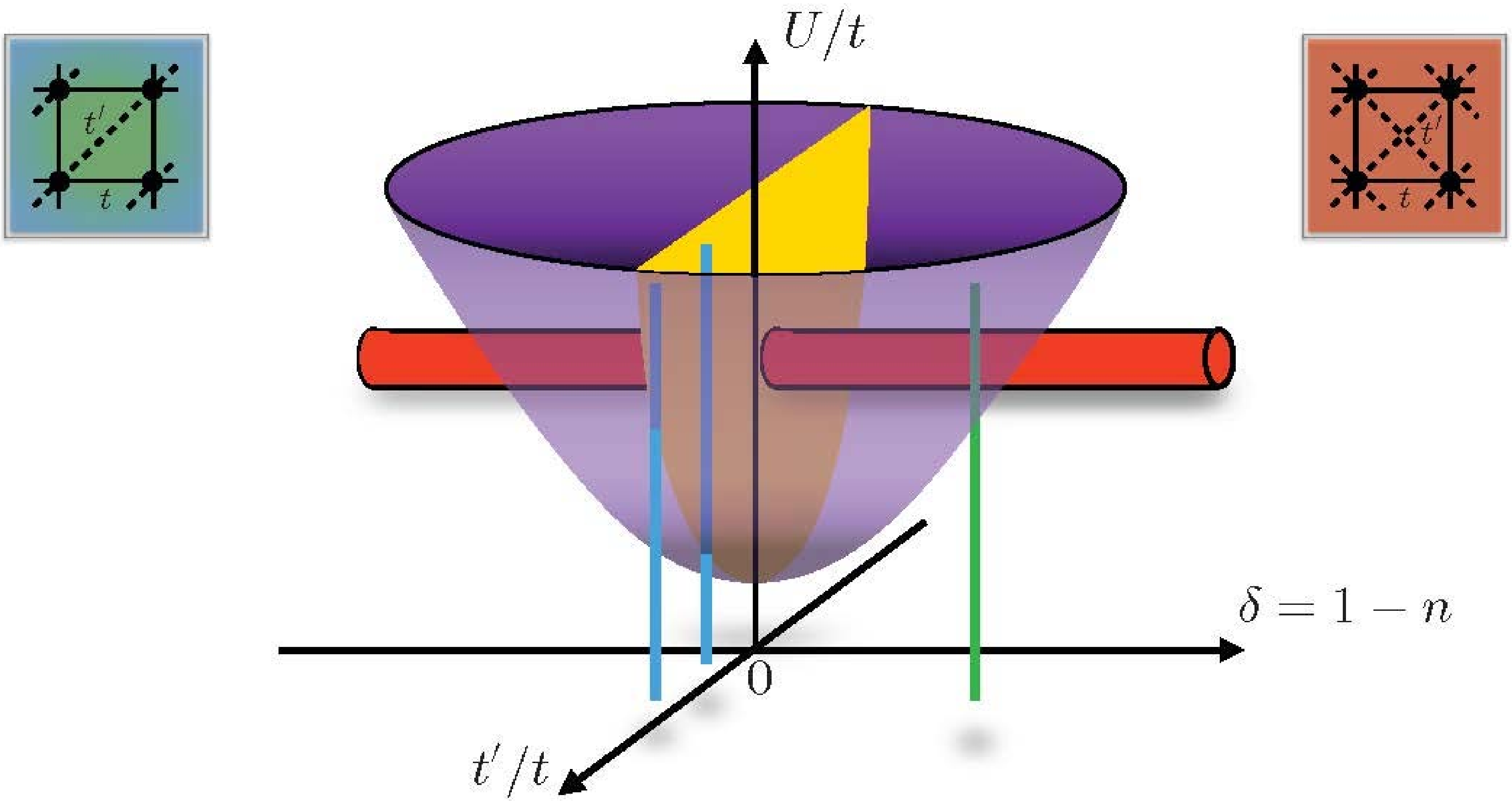
Perspective



Perspective



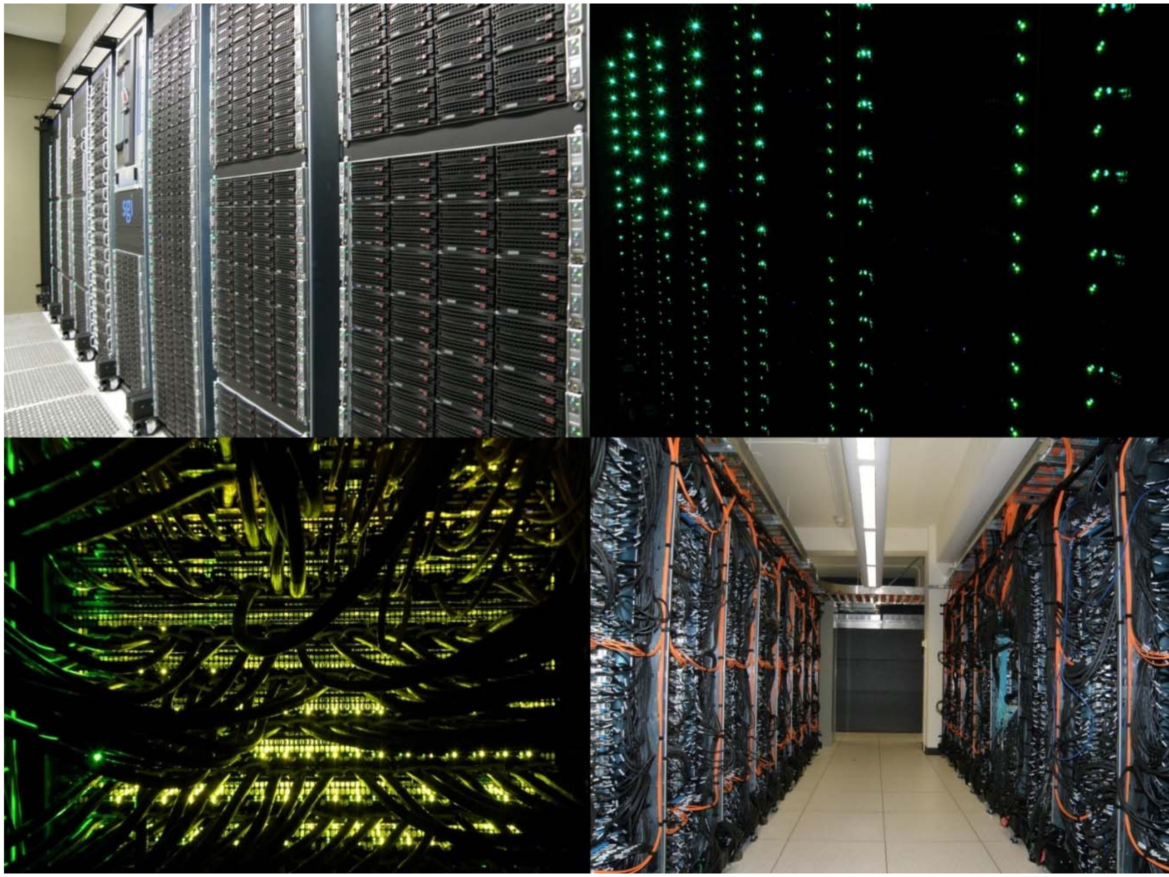
Perspective



Summary : organics

- Agreement with experiment
  - SC: larger T_c and broader *P* range if doped
  - Larger frustration: Decreases T_N *much more* than T_c
  - Normal state metal to pseudogap crossover
  - Effective mass increases towards Mott
  - Superfluid stiffness increases before fall near Mott
- Predictions
  - First order transition at low *T* in normal state (B induced)
  - Crossovers in SC state associated with normal state.
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range *J*.
  - T_c dome maximum near normal state 1st order

Mammouth



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Merci
Thank you

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