# Superconductivity beyond the dimer model in 2D organic charge transfer salts

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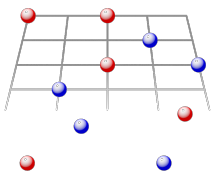
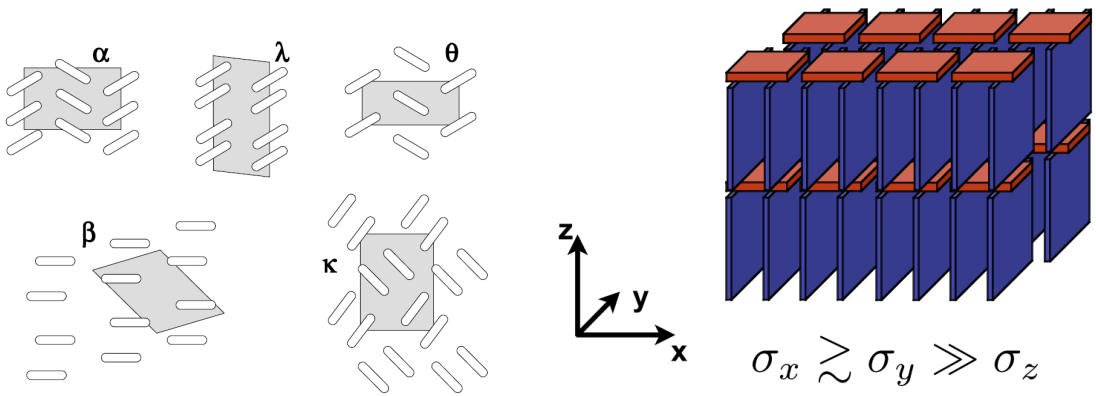
March 5, 2015

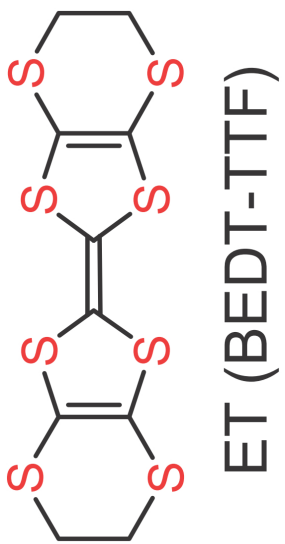


SFB/TR 49

# Organic charge transfer salts: Crystal structure and properties of $(ET)_2X$

- ET = BEDT-TTF = bis(ethylene-dithio)-tetrathiafulvalene is the electron donor
- X is the electron acceptor (e.g. $Cu(NCS)_2$)
- we concentrate on $\kappa$-$(ET)_2X$ salts
- AFI to SC transition with pressure or variation of X



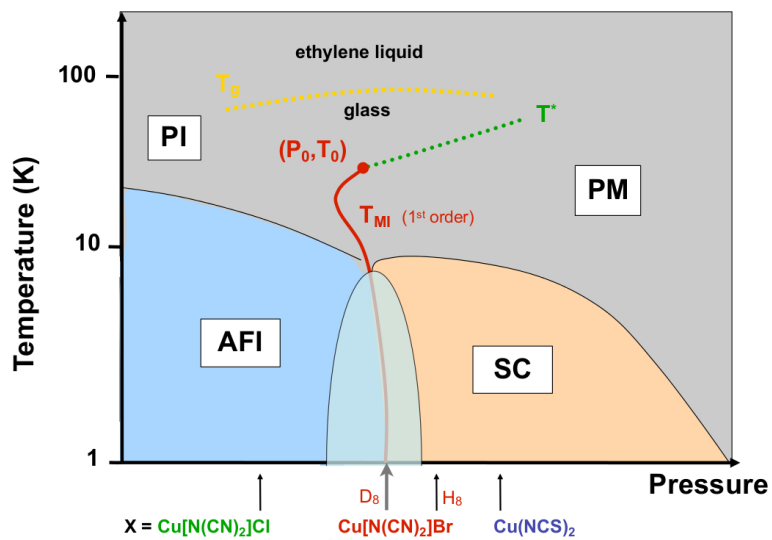




Figure : Müller, ChemPhysChem **12**, 1222 (2011)

# Organic charge transfer salts: Electronic structure of κ-$(ET)_2X$

- two donor molecules transfer in total one electron to the acceptor X
- two-dimensional electronic structure in the ET-plane
- four ET molecules in the unit cell, 3/4 filled four-band model
- effective model only describes dimers of ET molecules, 1/2 filled two-band model

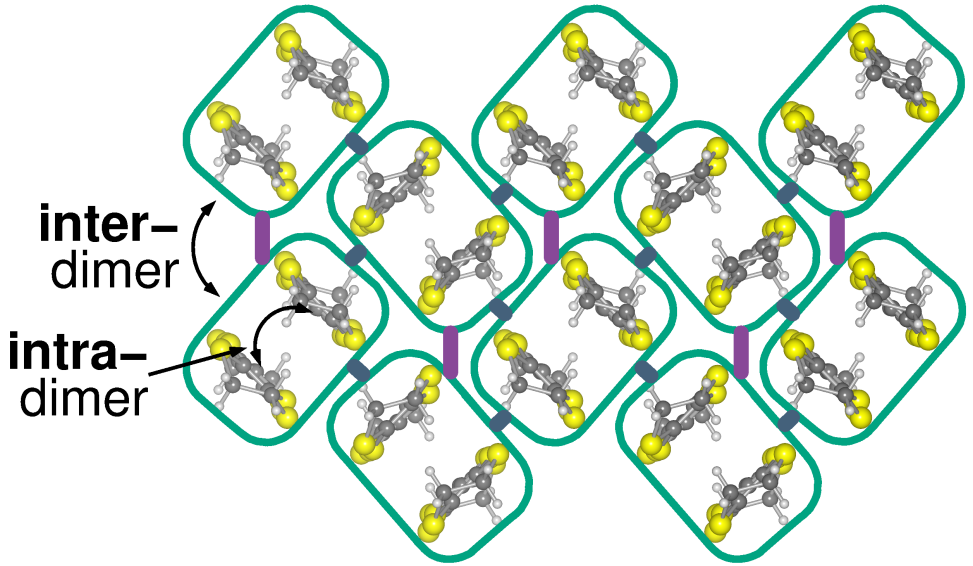



Figure : Ferber, Foyevtsova, Jeschke, Valentí, PRB **89**, 205106 (2014)

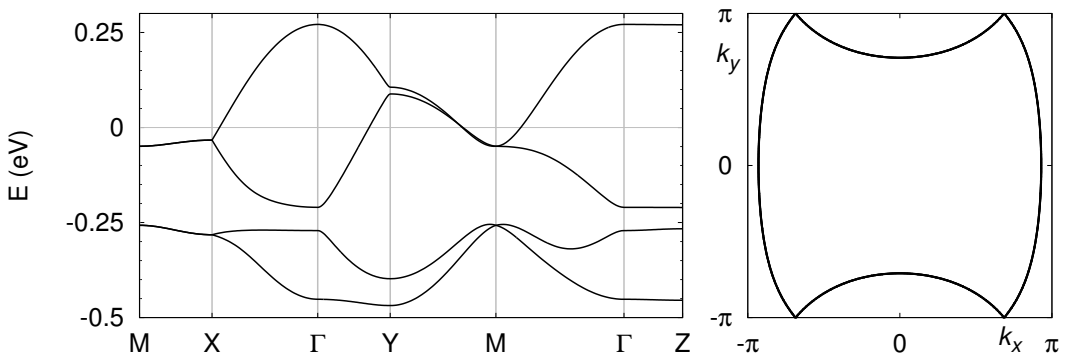



Figure : κ-$(ET)_2Cu(NCS)_2$

# Symmetry of superconducting pairing in κ-$(ET)_2X$

## *Ab-initio* calculations

- full potential local orbital (FPLO) code
- molecular orbital models from projective Wannier functions

## Superconductivity calculations

- RPA spin-fluctuation pairing

  Bickers, Scalapino, White, PRL **62**, 961 (1989)

  Graser, Maier, Hirschfeld, Scalapino, New J. Phys. **11**, 025016 (2009)

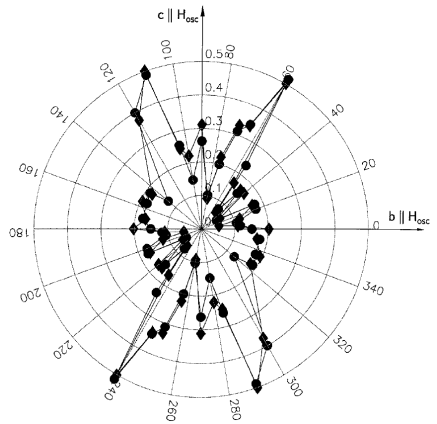
- extract pairing symmetry and relative strength

see also Schmalian, PRL **81**, 4232 (1998)

κ-$(ET)_2Cu(NCS)_2$

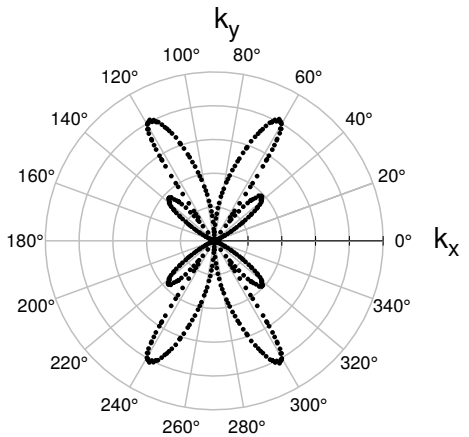
Experiment

Schrama *et al.*, PRL **83**, 3041 (1999)




Theory

Altmeyer, Guterding, Jeschke, Valentí, to be published

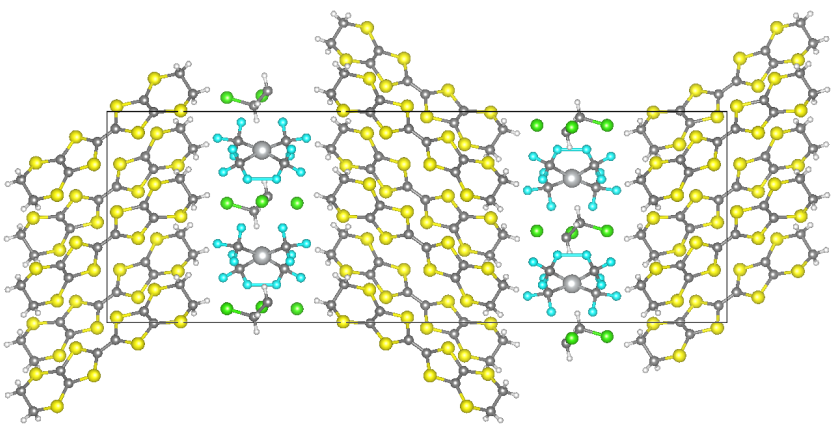


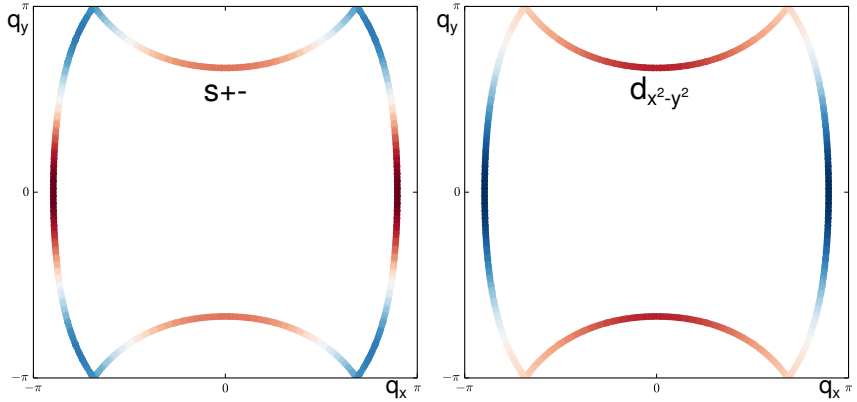

$d_{xy}$ from experiment and theory

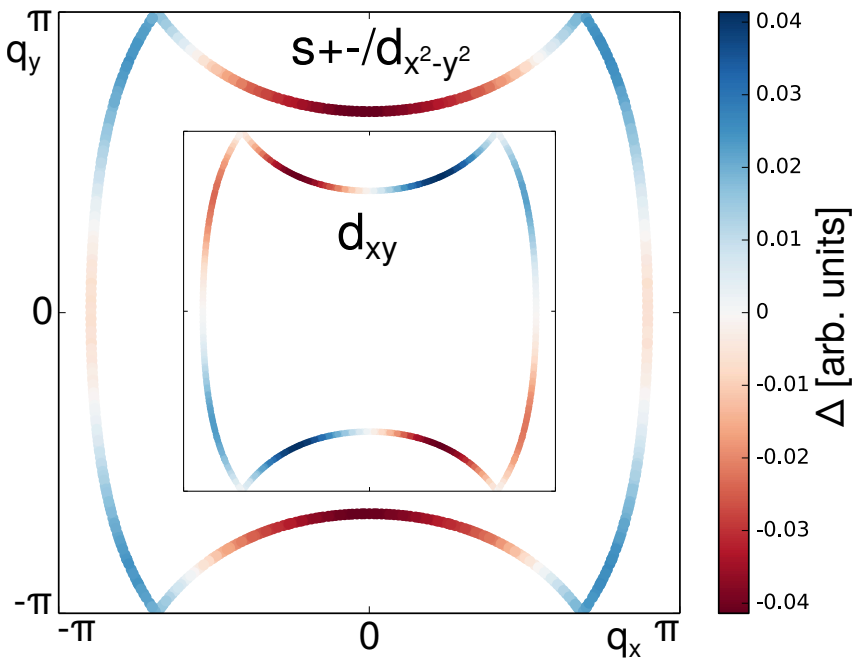
# Competing pairing symmetries in κ-$(ET)_2X$

## κ-$(ET)_2Ag(CF_3)_4(TCE)$

- leading eigenfunction: 71% s±, 29% $d_{x2-y2}$
- subleading: 100% $d_{xy}$



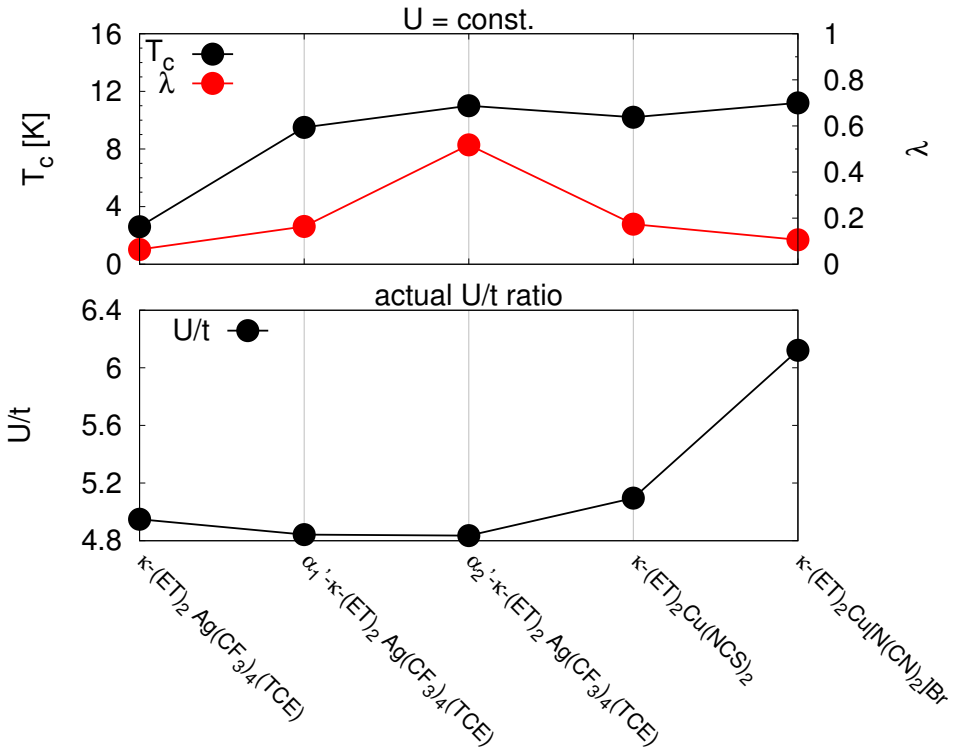


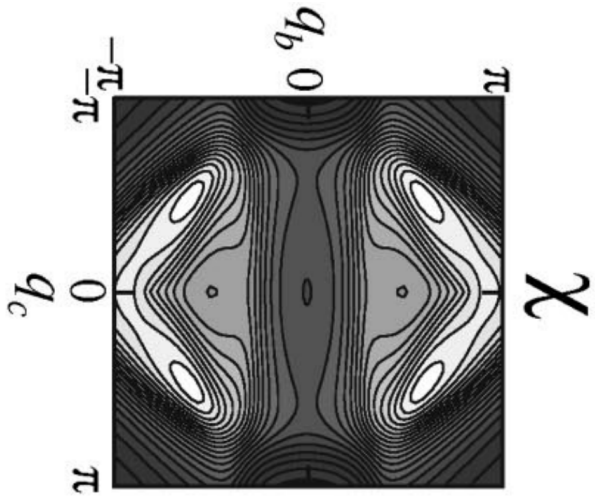

see also Schmalian, PRL **81**, 4232 (1998); Kuroki *et al.*, PRB **65**, 100516(R) (2002)

# Material dependence of $T_c$ in $\kappa$-$(ET)_2X$

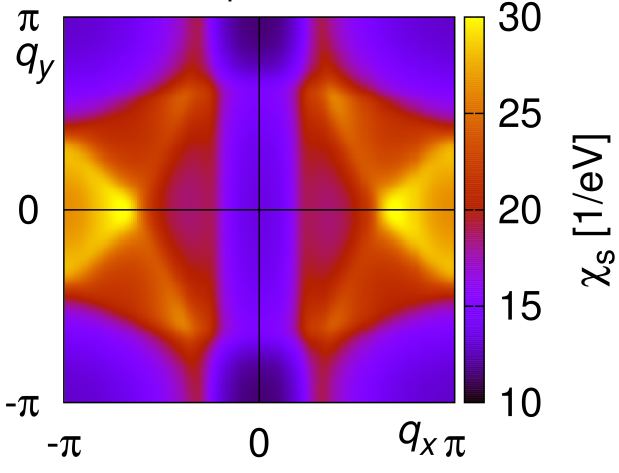
- $\lambda$ measures pairing strength
- $U$ is material dependent
- feature rich spin-susceptibility not discussed in previous work




Kuroki *et al.*, PRB **65**, 100516(R) (2002)




Altmeyer, Guterding, Jeschke, Valentí, to be published



## Summary

- we derived *ab-initio* models for many κ-phase materials
- RPA spin-fluctuation pairing yields $s_{\pm}/d_{x^2-y^2}$ or $d_{xy}$ gap
- material dependence of $T_c$ comes out correctly
- no simple dependence on microscopic parameters

Altmeyer, Guterding, Jeschke, Valentí, to be published

# Conversion from four-band to dimer model

- $t = \frac{1}{2}(t_2 + t_4)$
- $t' = \frac{1}{2}t_3$
- $U = 2t_1$

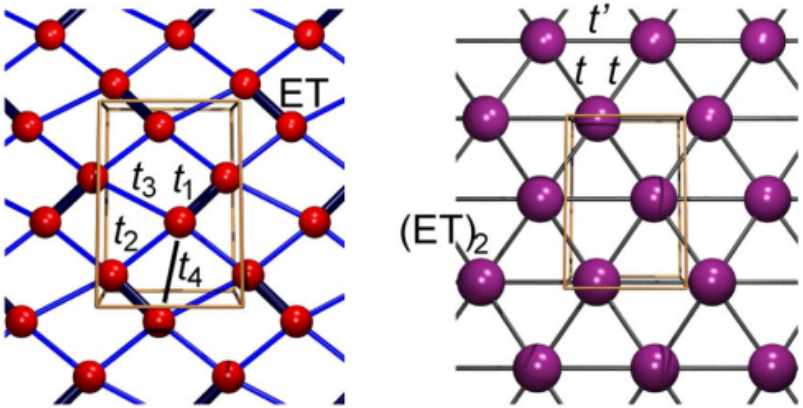



Figure : Kandpal et al., PRL **103**, 067004 (2009)

# Tight binding+RPA formalism in a nutshell

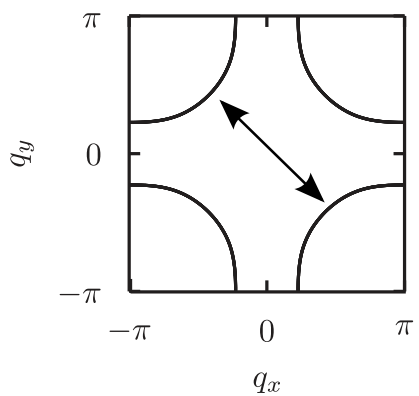
$$\chi^{pq}_{st}(\vec{q}) = -\frac{1}{N}\sum_{\vec{k},\mu,\nu} a^{s}_{\mu}(\vec{k})a^{p*}_{\mu}(\vec{k})a^{q}_{\nu}(\vec{k}+\vec{q})a^{t*}_{\nu}(\vec{k}+\vec{q})\frac{f(E_\nu(\vec{k}+\vec{q})) - f(E_\mu(\vec{k}))}{E_\nu(\vec{k}+\vec{q}) - E_\mu(\vec{k})}$$

$$\left[(\chi^{RPA}_{spin})^{pq}_{st}\right]^{-1} = \left[\chi^{pq}_{st}\right]^{-1} - (U_{spin})^{pq}_{st}$$

$$\Gamma^{pq}_{st}(\vec{k},\vec{k}') = \left[\frac{3}{2}U_s\,\chi^{RPA}_{s}(\vec{k}-\vec{k}')\,U_s + \frac{1}{2}U_s - \frac{1}{2}U_c\,\chi^{RPA}_{c}(\vec{k}-\vec{k}')U_c + \frac{1}{2}U_c\right]^{tq}_{ps}$$

$$\Gamma_{ij}(\vec{k},\vec{k}') = \sum_{stpq} a^{t*}_{i}(-\vec{k})a^{s*}_{i}(\vec{k})\mathrm{Re}\left[\Gamma^{pq}_{st}(\vec{k},\vec{k}')\right]a^{p}_{j}(\vec{k}')a^{q}_{j}(-\vec{k}')$$

$$-\sum_{j}\oint_{C_j}\frac{dk'_{\parallel}}{2\pi}\frac{1}{4\pi v_F(\vec{k}')}\left[\Gamma_{ij}(\vec{k},\vec{k}') + \Gamma_{ij}(\vec{k},-\vec{k}')\right]g_j(\vec{k}') = \lambda_i g_i(\vec{k})$$




- Graser, Maier, Hirschfeld, Scalapino, New Journal of Physics **11**, 025016 (2009)

# Other interesting talks

- talk after next one : Electronic structure of a dual-layered organic charge transfer salt, Harald O. Jeschke
- **Z5.00004** : Generalized bandstructure unfolding method, **Friday 11:15 AM**, Milan Tomić

# Summary of superconductivity calculations

- feature rich spin-susceptibility
- RPA spin-fluctuation pairing yields $s_{\pm}/d_{x^2-y^2}$ or $d_{xy}$ gap
- material dependence of $T_c$ comes out correctly
- complicated dependence on microscopic parameters