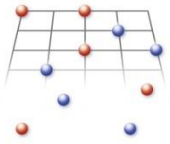
Excitations and Interactions

- Magnon gases **A7** **A8**
- Spin physics **A3** **A5** **A9** **A10** **A12**
- Quantum magnets **A3** **A8** **B1** **B2** **B3** **B4** **B5**
- Synthesis **B4** **B6** **B9** **$B10_E$**
- Spectroscopy **B8** **B9** **B11** **B12**



Excitations and Interactions

Real Systems

- Charge-transfer induced changes in orbital occupation

  NEXAFS

  B8 B10$_E$ B12 B4 B2

- Core-level shift at the charge-order transition

  HAXPES

  B8 B12 B6 B4

- Many-body effects and density of states near E_F

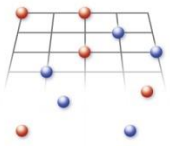
  STS

  B12 B11 B9 B8 B6

- Anisotropic strain in ferroelectric CT system

  CS

  B9 B8

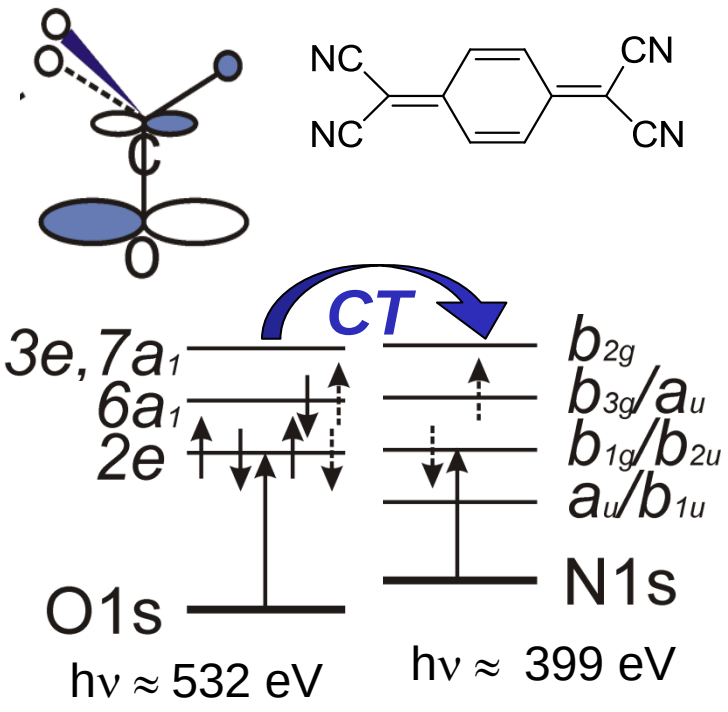


Excitations and Interactions

- Charge-transfer induced changes in orbital occupation

Near-edge X-ray absorption fine structure (***NEXAFS***)

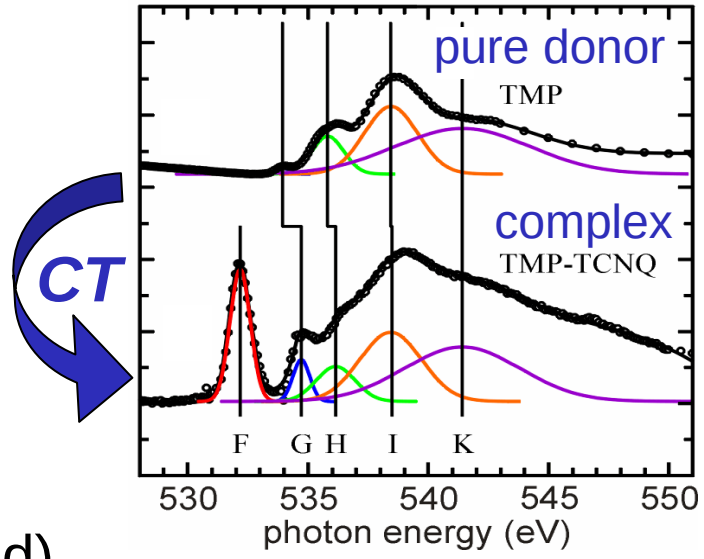
B8 **B10$_E$** **B12** **B4** **B2**



Tuneable soft X-rays

@ ANKA (Karlsruhe); MAXLAB (Lund)

Element-specific probe of unoccupied states



JACS **134**, 4694 (2012)

NEXAFS on novel organic charge-transfer complexes

Highlight: Novel CT-complexes based on pyrene derivatives or DTBDT with TCNQ

- CT-complex UHV-deposited and solution-grown crystallites
- Theory explains shifts of donor and acceptor orbitals

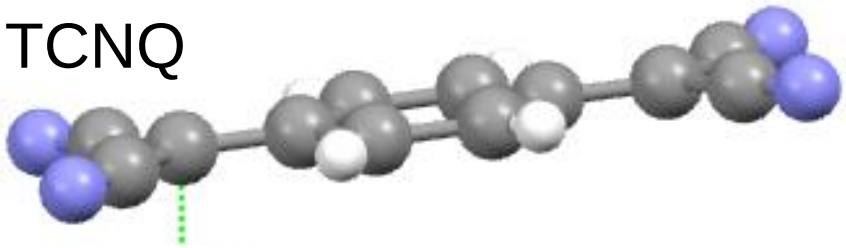
Tetramethoxypyrene-TCNQ JACS **134**, 4694 (2012)

***TTF-TCNQ:* CDW instability** Eur. Phys. J. B **88, 13** (2015)

with J.-P. Pouget (Orsay) and E. Canadell (Barcelona)

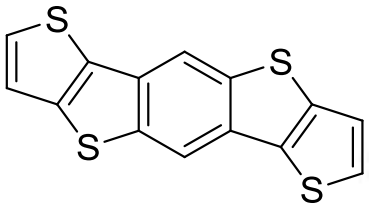
B8 **$B10_E$** **B12** **B2** **B4**

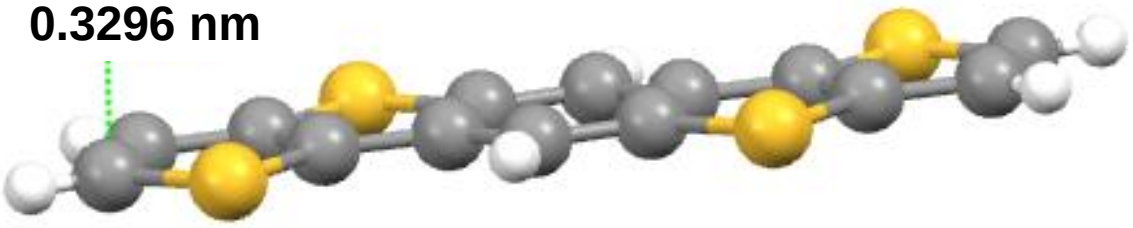
TCNQ

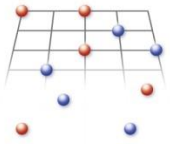


0.3296 nm

DTBDT





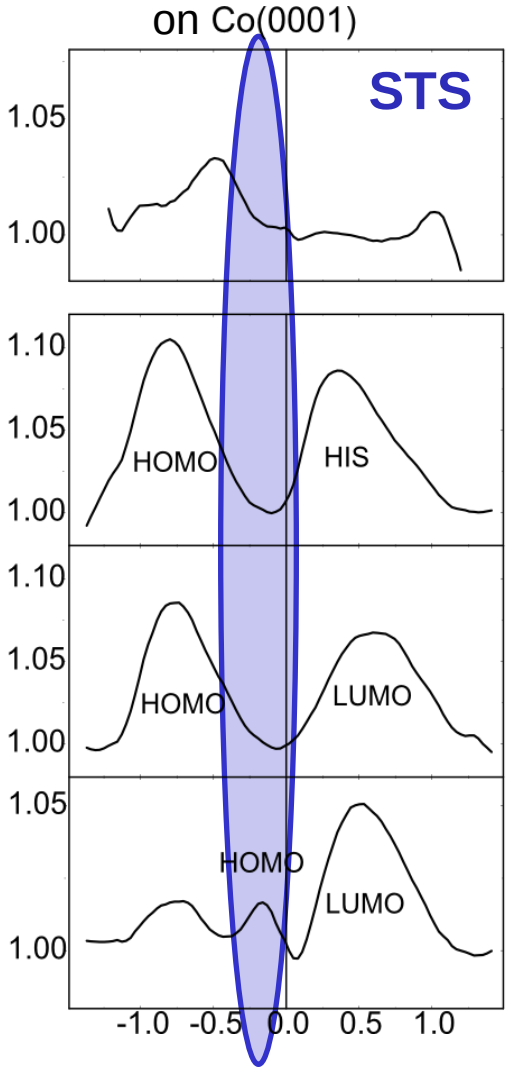


Transregio 49
Frankfurt / Kaiserslautern / Mainz

Extremely short interplanar C-C distances < 0.33 nm,
very short S-S contacts ~ 0.34 nm

Charge-transfer state in DTBDT close to the Fermi level

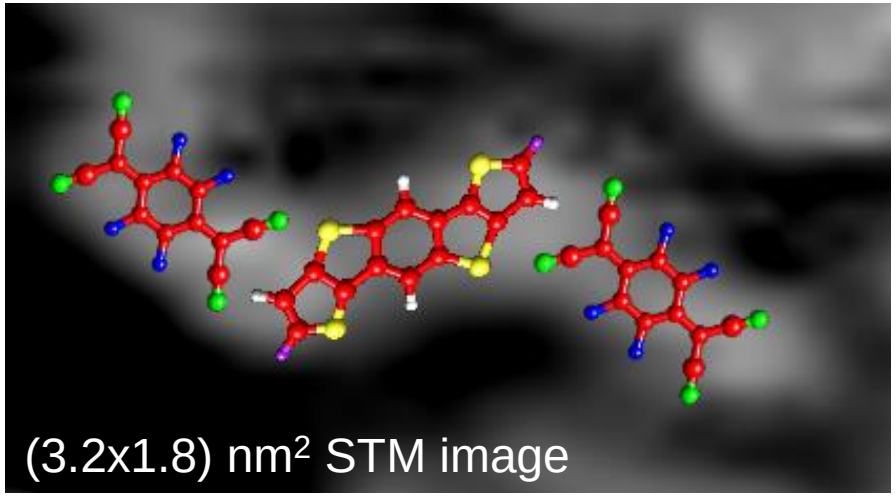
PRB **89**, 075435 (2014)

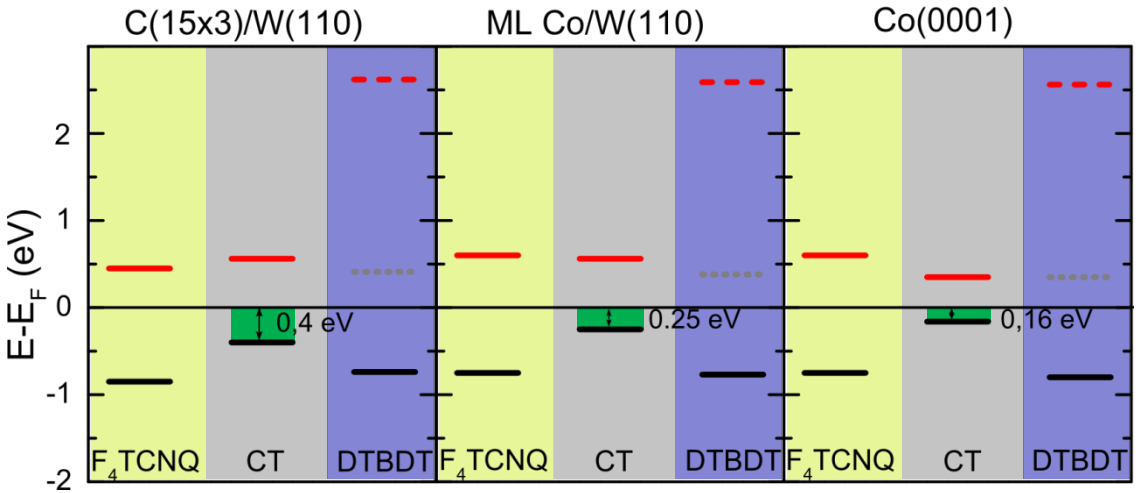


B12

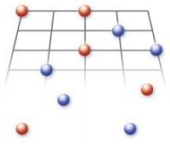
B10$_E$

B4





Split HOMO state in DTBDT-F_4TCNQ -compound indicates charge transfer



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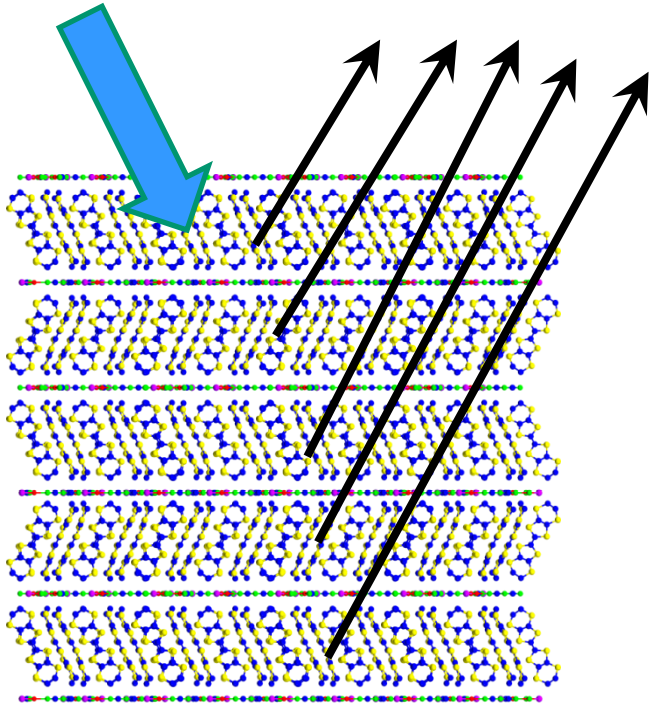
Excitations and Interactions

- Core-level shift at the CO transition

B8 **B10** **B12** **B6** **B4**

Hard X-ray photoemission (*HAXPES*) @ PETRA III

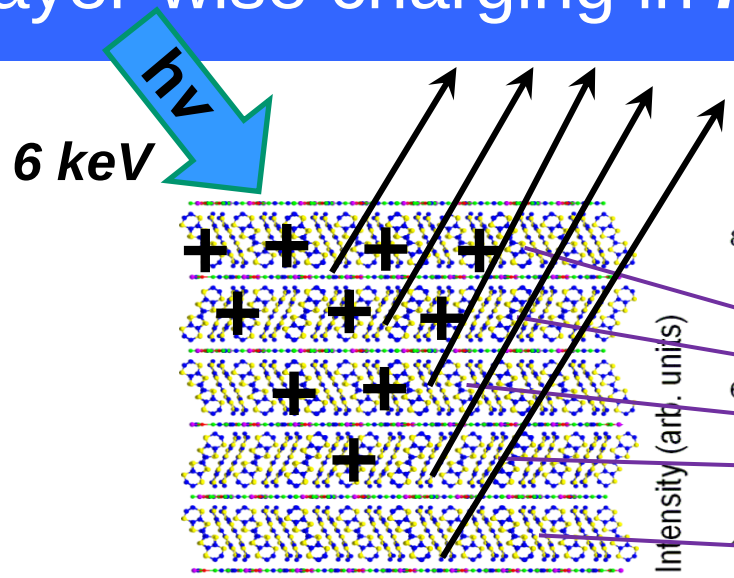
hν =
6-10 keV

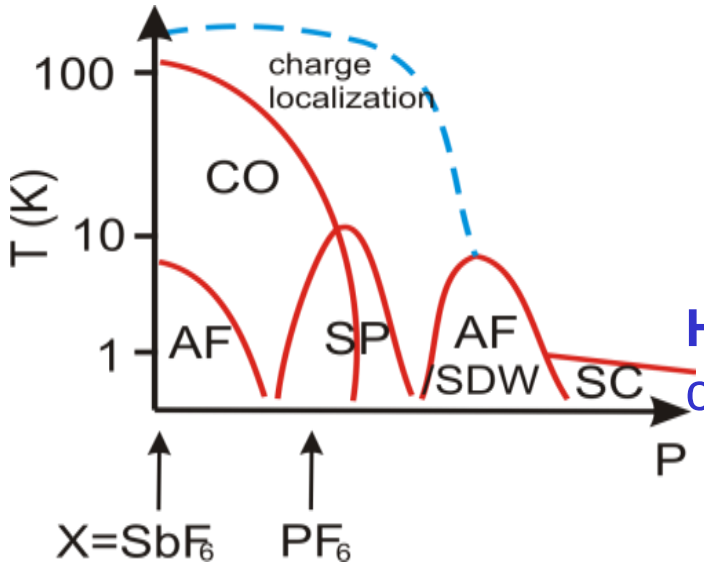


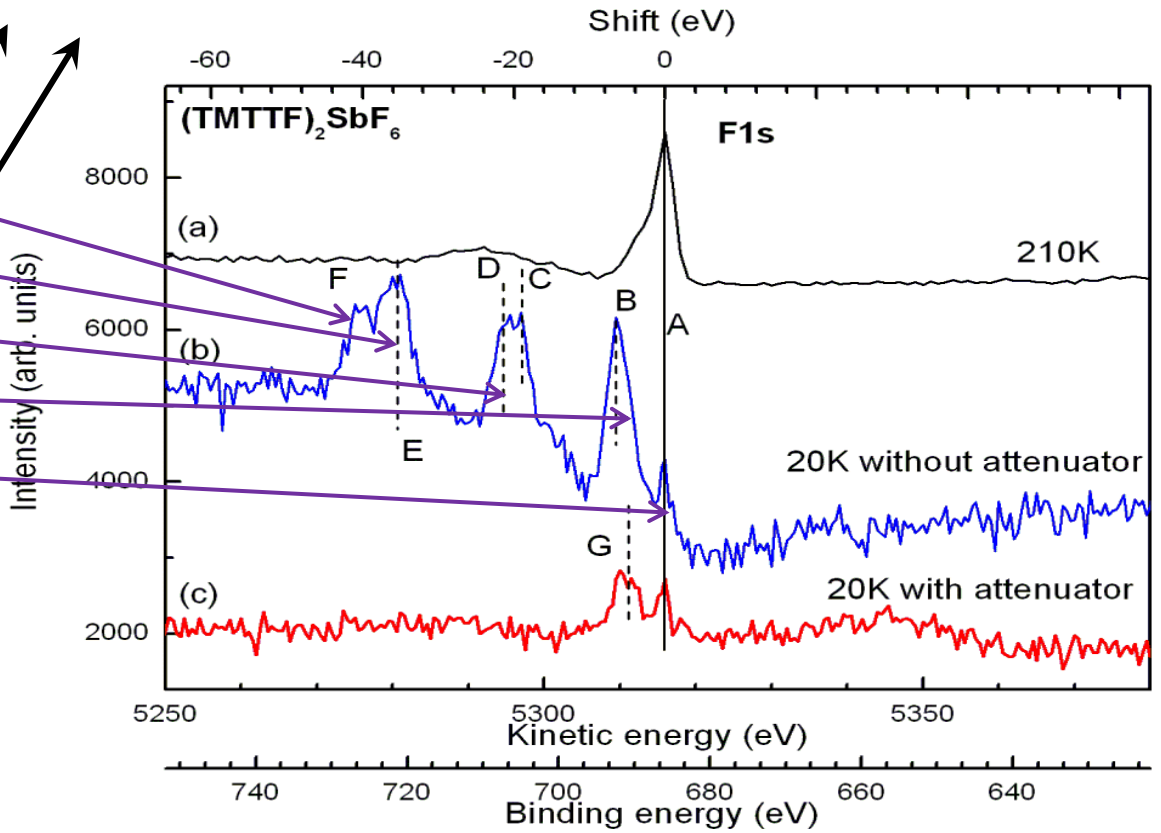
15 - 20 nm escape depth

Bulk-sensitive photoemission

Layer-wise charging in ***HAXPES*** uncovered and solved







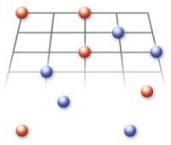
Highlight: HAXPES detecting chemical shift at charge-order transition in Fabre salt $(TMTTF)_2SbF_6$

- clarifying mechanism of anomalous charging
- detecting true chemical shift

B 8 **B 6** **B11** **B12**

Eur. Phys. J. B **87,** 256 (2014)

with J.-P. Pouget (Orsay)



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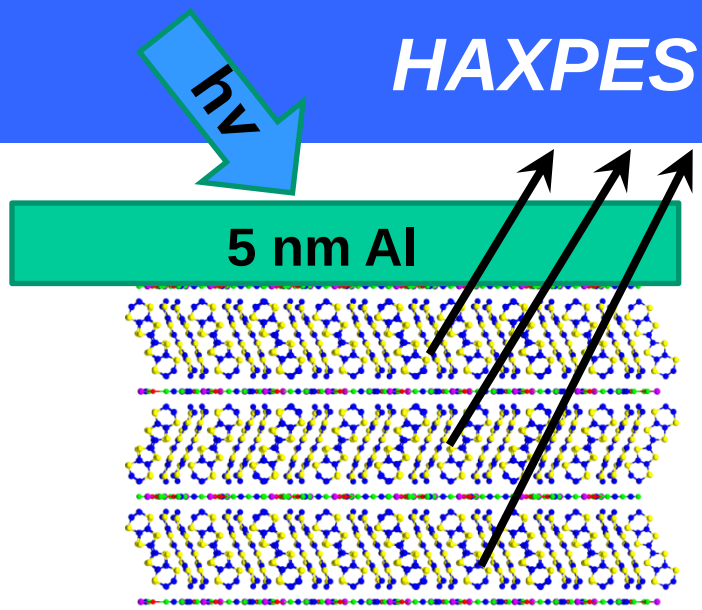
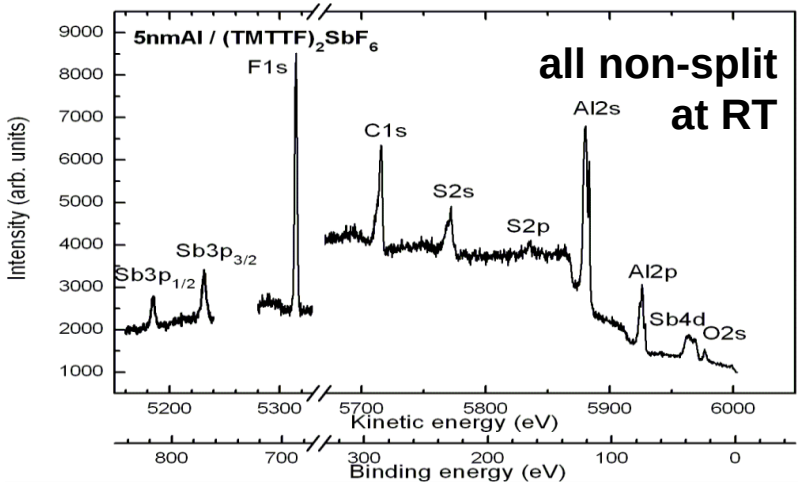
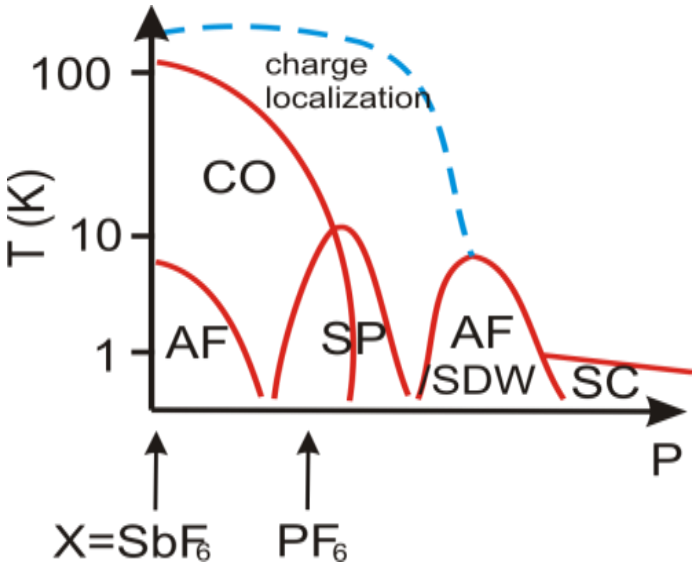
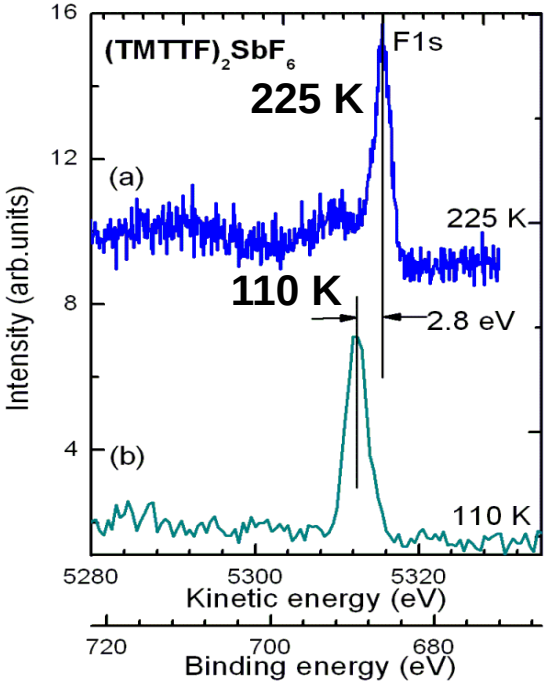
HAXPES on Fabre salt $(TMTTF)_2SbF_6$





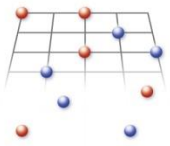




F 1s core level shift:
fingerprint of
displacement of anions
at the CO transition.

B 8 **B 6** **B11** **B12**

Eur. Phys. J. B **87,** 256 (2014)
with J.-P. Pouget (Orsay)



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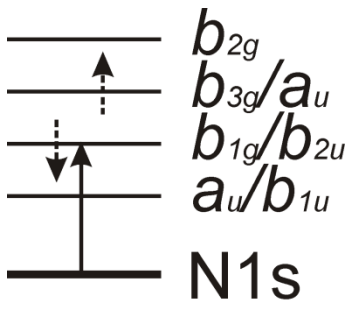
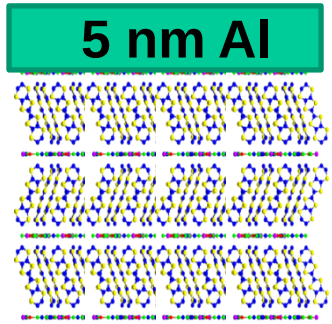
Resumé on ***Electron & X-ray Spectroscopy***

***NEXAFS*: excitation in „neutral complex“**

***HAXPES*: Look through metal coating**

Radiation damage is an issue !





Resumé on ***Electron & X-ray Spectroscopy***

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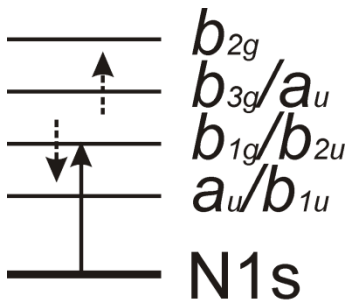
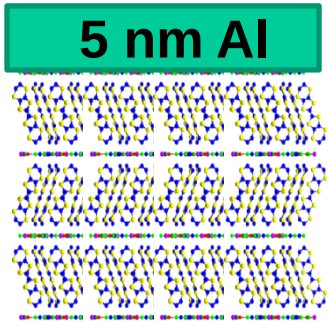
Radiation damage is an issue !

B8 Next:

k-microscopy

→ extremely low radiation dose





Excitations and Interactions

Real Systems

- Charge-transfer induced changes in orbital occupation

  NEXAFS

  B8 B10$_E$ B12 B4 B2

- Core-level shift at the charge-order transition

  HAXPES

  B8 B12 B6 B4

- Many-body effects and density of states near E_F

  Scanning Tunnelling Spectroscopy ***STS***

  B12 B8 B6

- Anisotropic strain in ferroelectric CT system

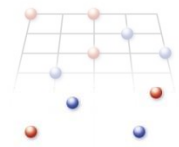
  Conductivity spectroscopy

  B9 B8

- Excitations in magnonic systems

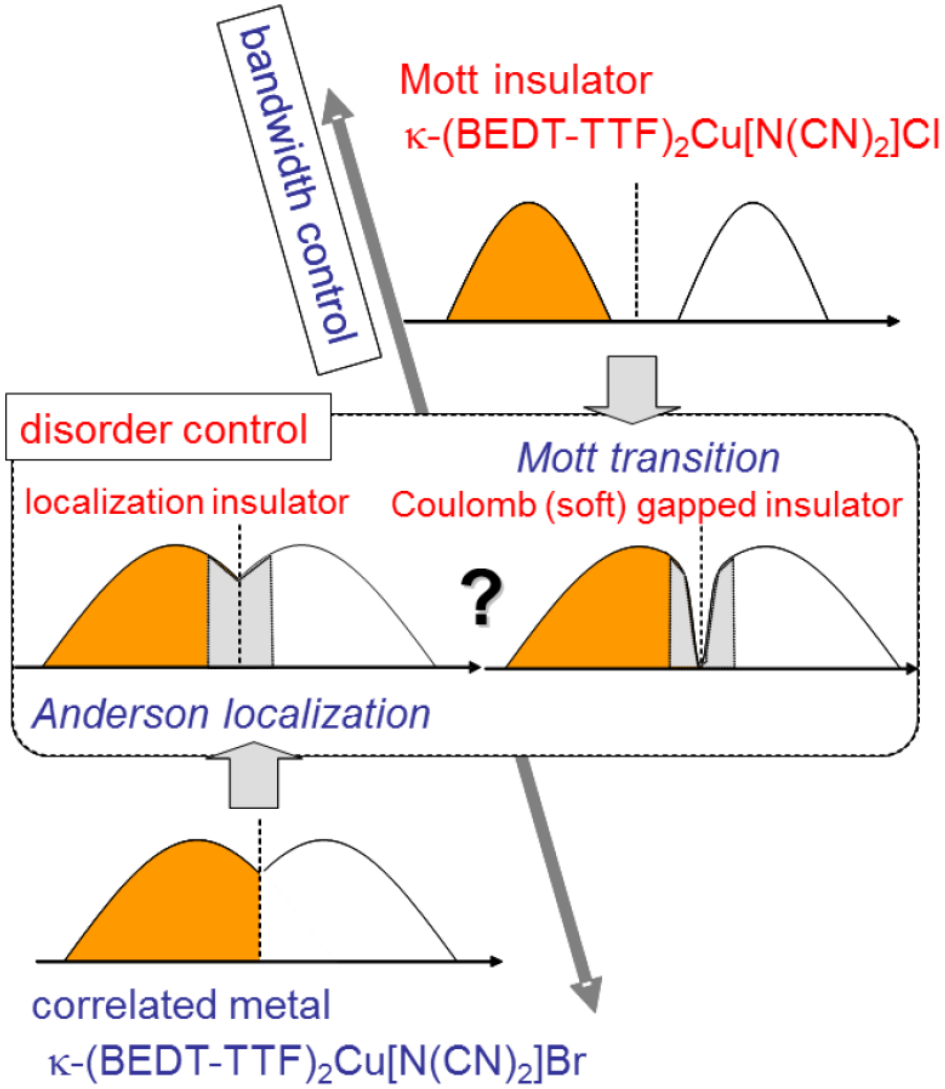
  Brillouin spectroscopy

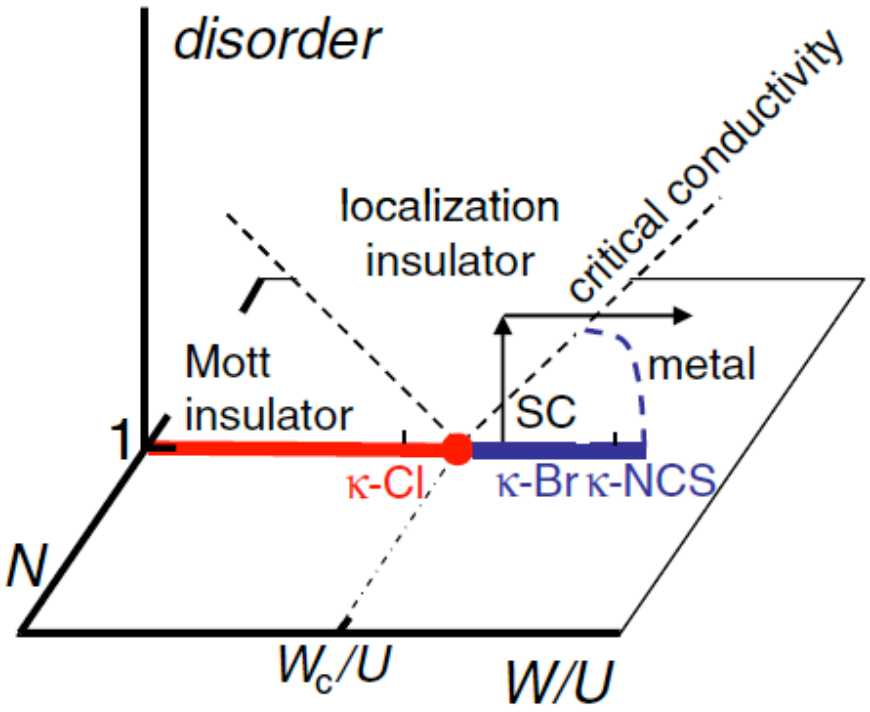
  A7



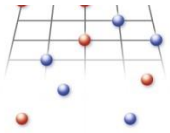
Electron correlation in organic CT salts probed by ***STS***

B12 **B2** **B6** **B9** **B11**





T. Sasaki et al., PRL 2010



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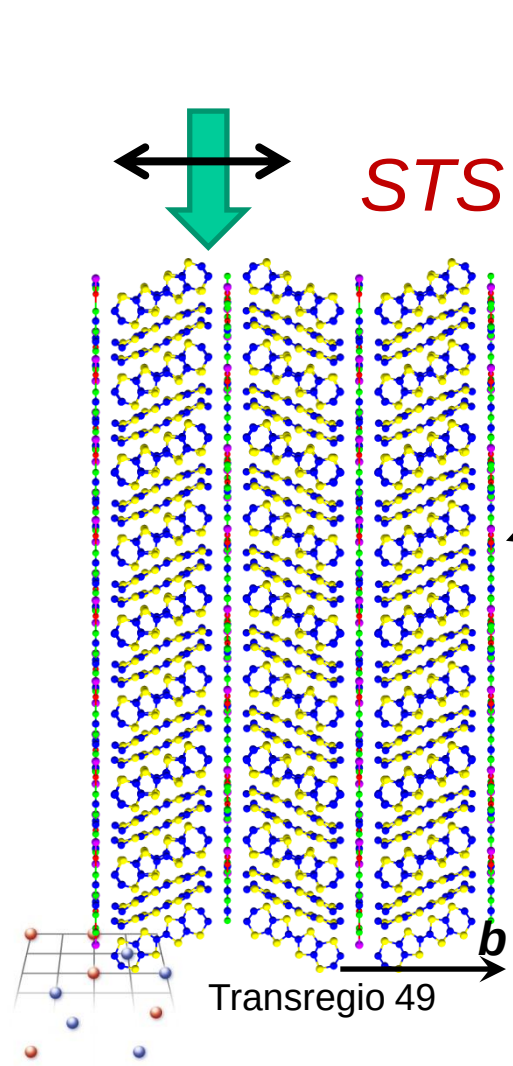
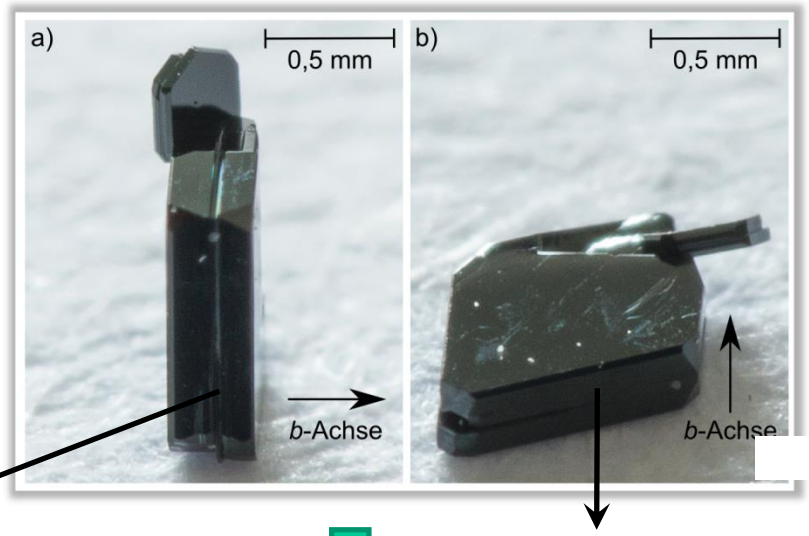
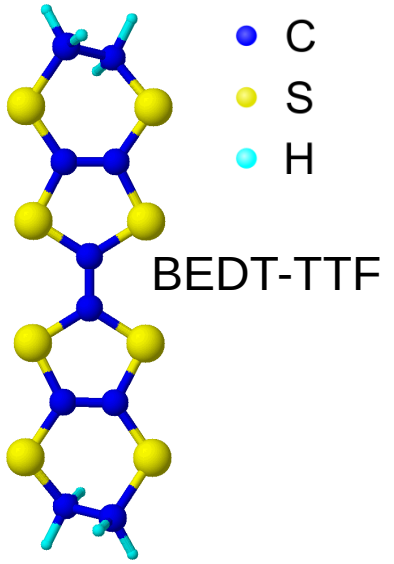
Electron correlation in organic CT salts probed by ***STS***

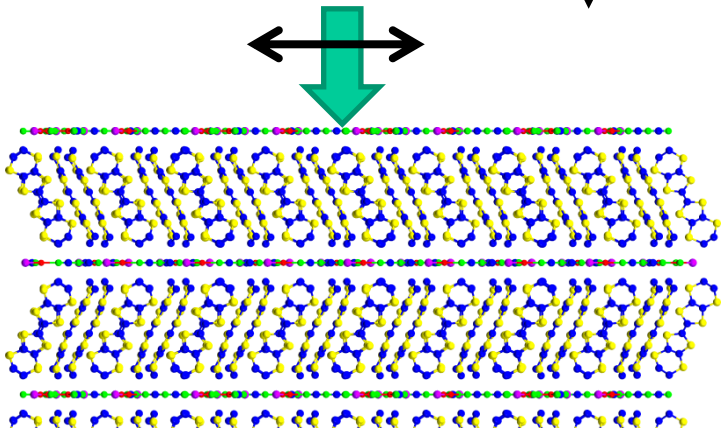
- Study electronic properties of CT systems with lateral resolution
- Many-body effects and density of states near Fermi energy
- Investigate new charge transfer systems with electronic correlation

B12 **B6** **B9** **B11**

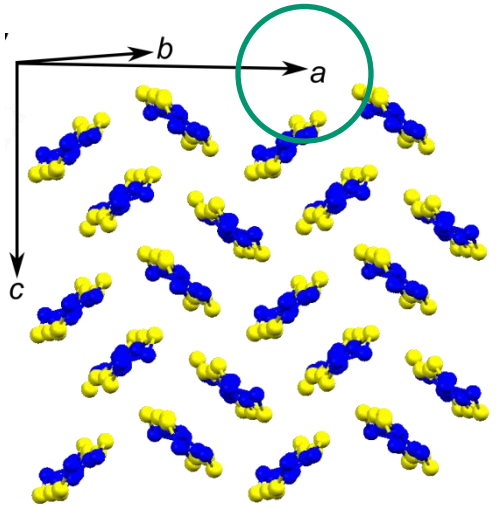






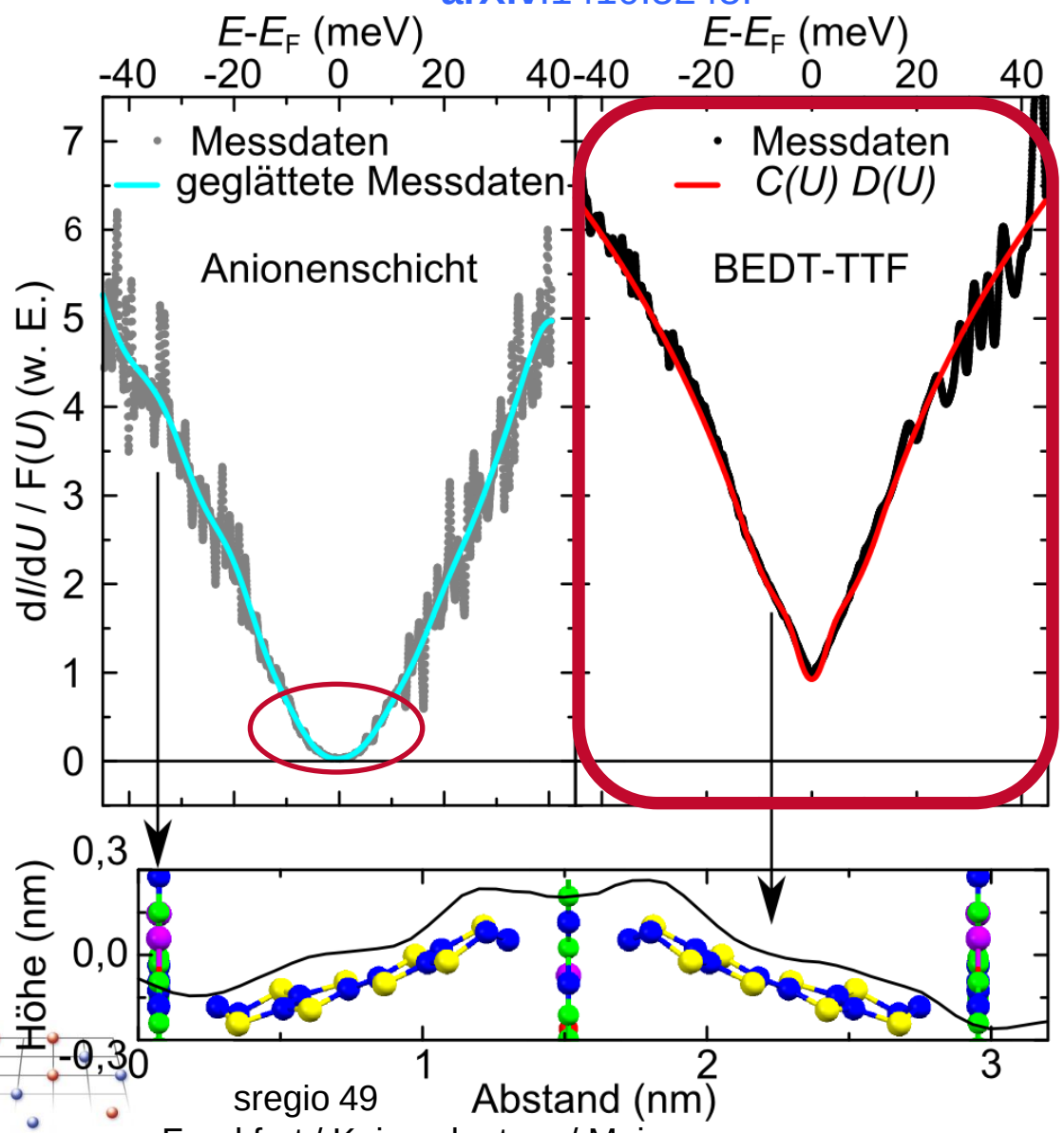


κ-(BEDT-TTF)$_2$ Cu[N(CN)$_2$]Br



Electron correlation in organic CT salts probed by ***STS***

arXiv:1410.5245.

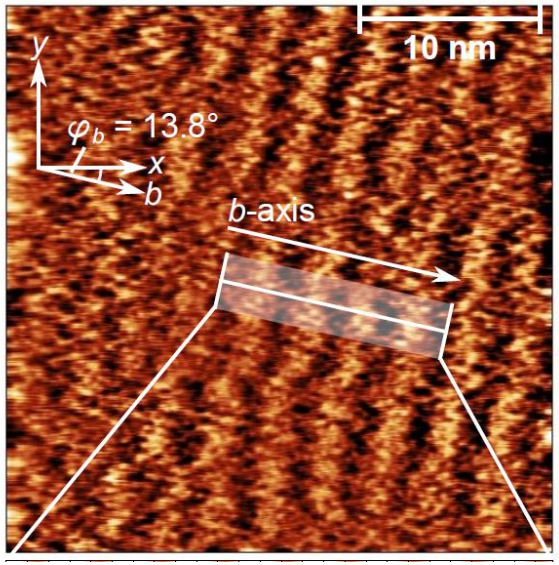


Anion layer:

- DOS = 0 at E_F
- Energy gap of DOS
- Insulating behavior

BEDT-TTF-layer:

- Finite DOS at E_F
- V-shaped DOS

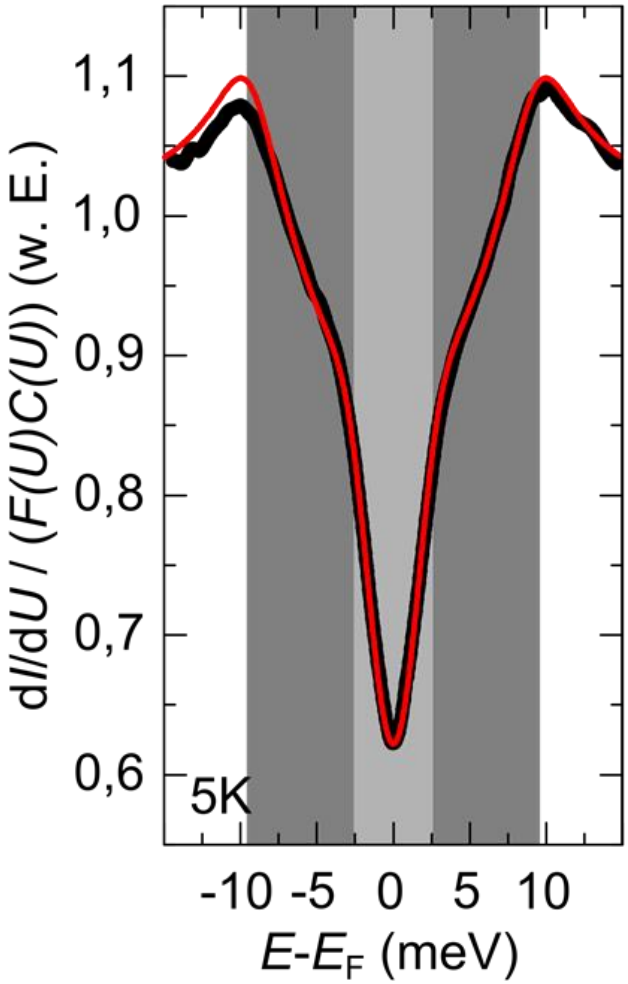


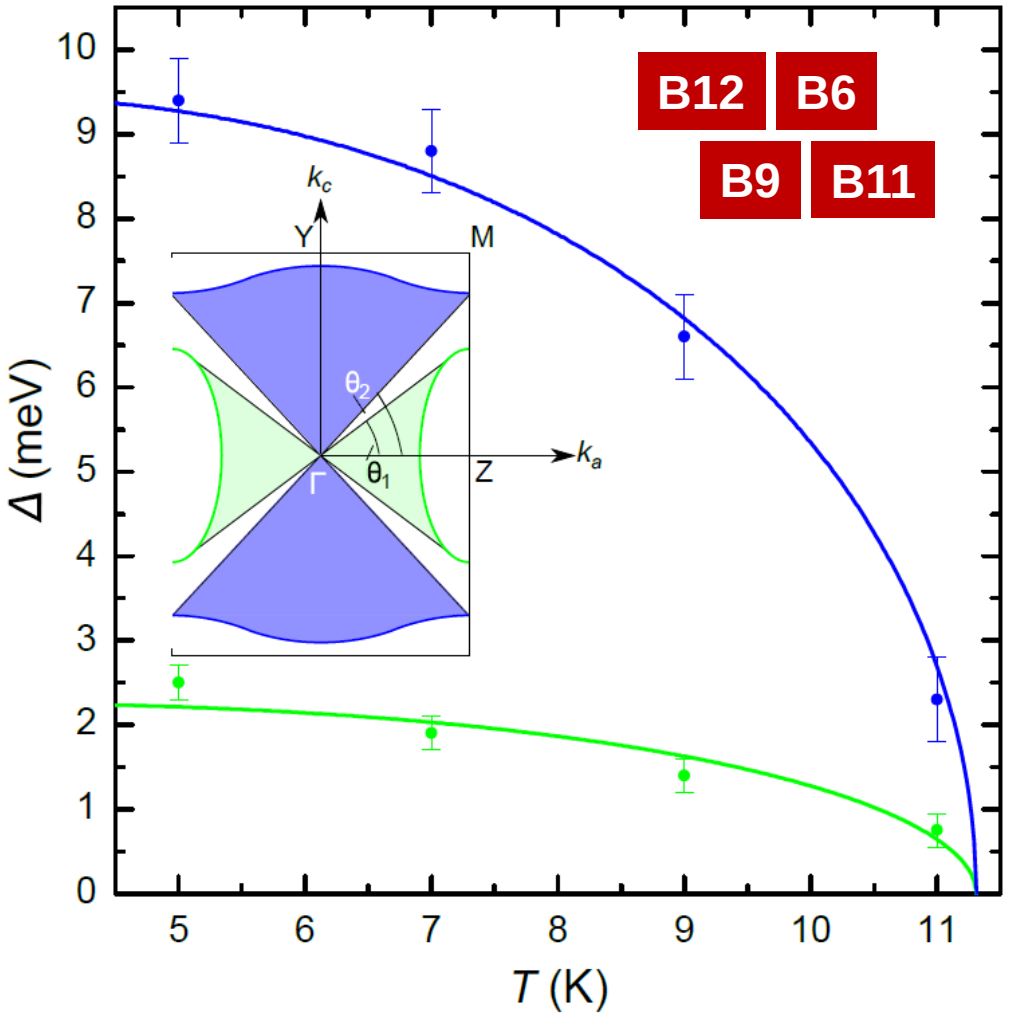
Soft gap → Anderson localization

B12 B6 B9 B11

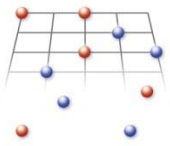
Electron correlation in organic CT salts probed by ***STS***

Highlight: Two gap superconducitivity in κ-Br **arXiv:** 1411.2813





Both gaps vanish at the same critical temperature
→ strong interband coupling



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Electron correlation in organic CT salts probed by ***STS***

Next: **B12**

- Anderson localization for k-ET2-X varied by

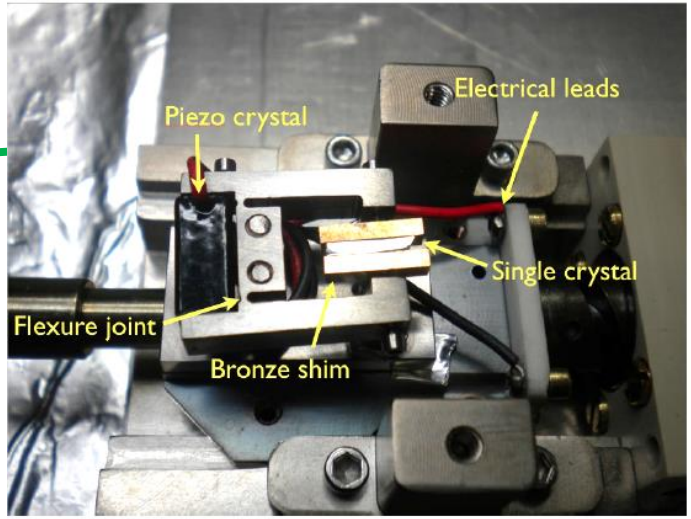
  rapid cooling

  X-ray irradiation

- Bandwidth modulation by

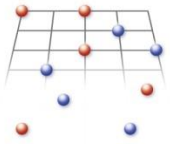
  uniaxial pressure

  D8-H8 disorder



Courtesy of C.A. Jenkins, ALS

- Study of novel CT salts **B8** **B4**



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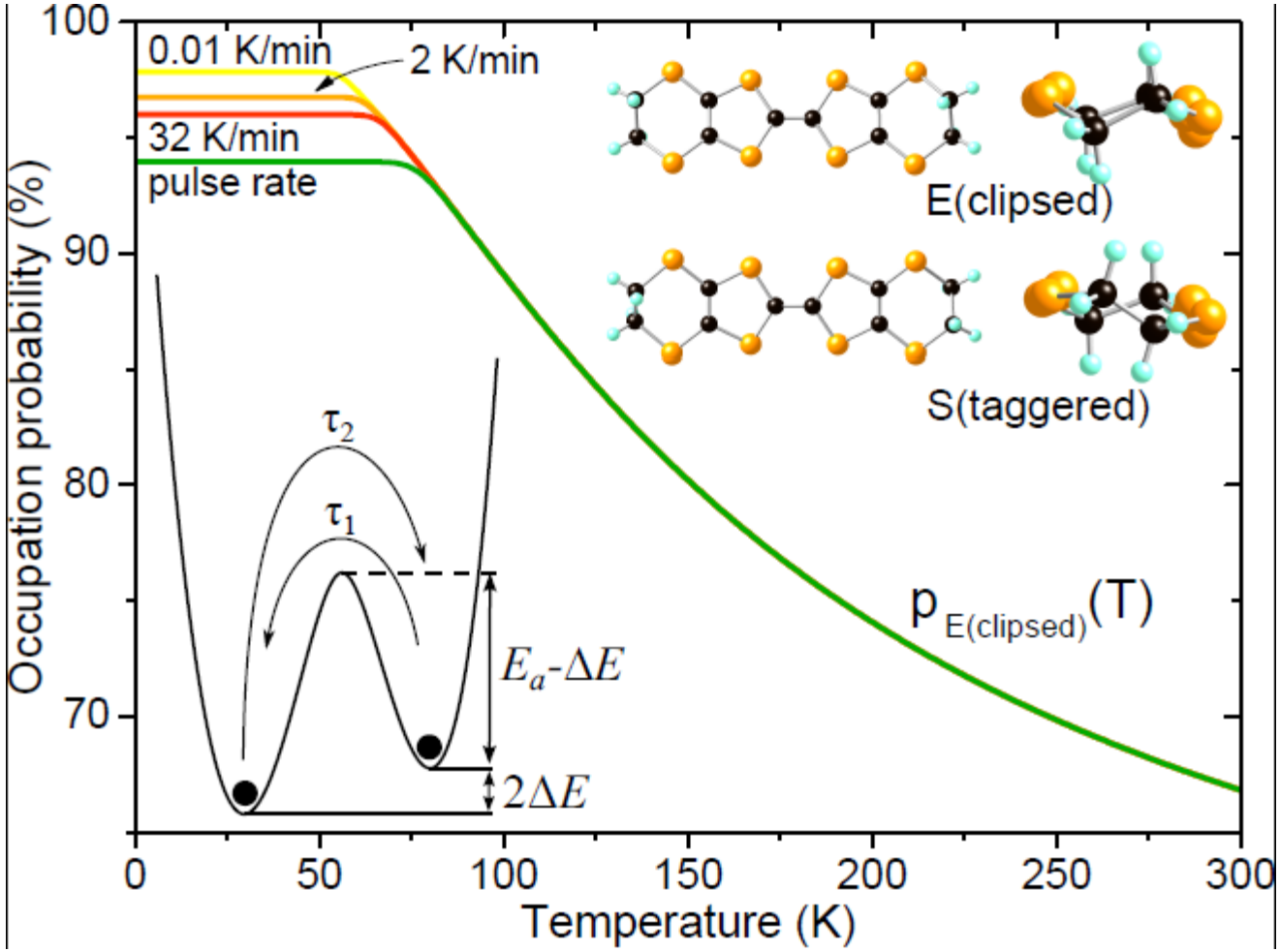
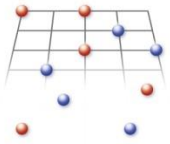
PRB **90**, 095150 (2014)





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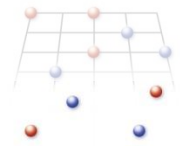


Thin film investigations of ***ferroelectric*** organic CT systems

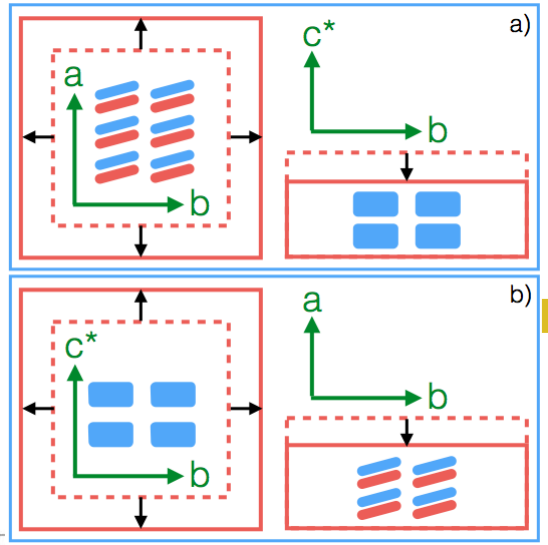
- Effects of anisotropic strain on ferroelectric state of mixed stack organic CTS ***TTF-QCl$_4$*** (neutral-ionic transition T_{NI})
- Degree of order-parameter coupling „dimerization“ - „charge transfer“?
- Long-range order in dimerized spin-chain of donor-acceptor stacks?

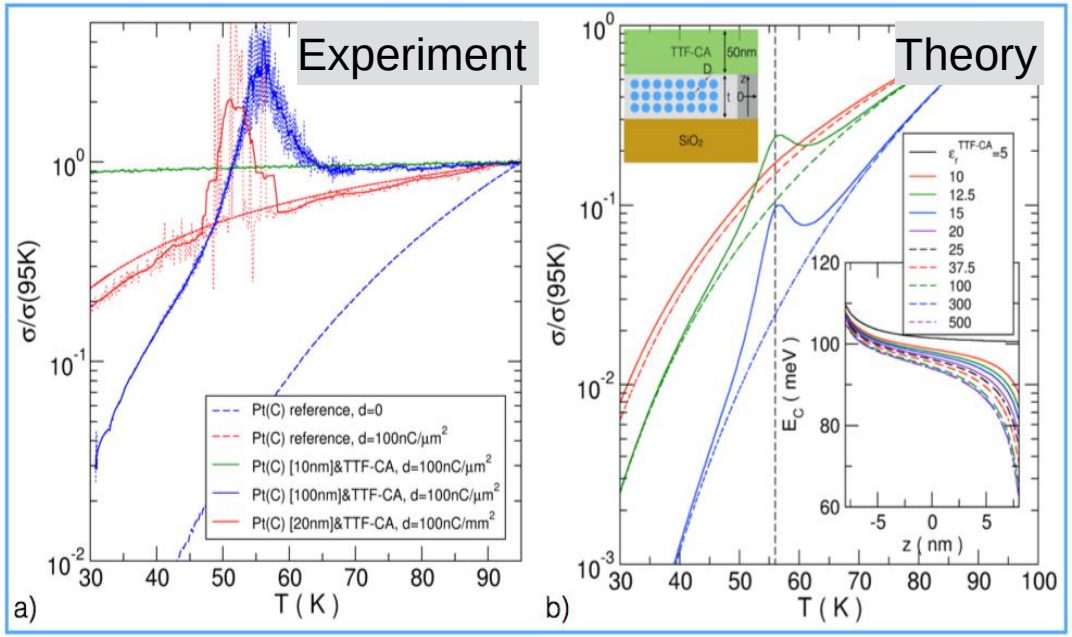
Highlights

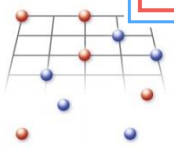
B9 **B8**

Mater. Res. Expr. **1**, 046303 (2014); Appl. Phys. A **117**, 1689 (2014)

- Thin film growth of *TTF-QCl$_4$* causes anisotropic strain ⇒ **Shift of T_{NI} by 30%**
- Non-invasive probing of ferroelectric transition by dielectric sensing in neighboring nano-granular metal layer (experiment & theory)







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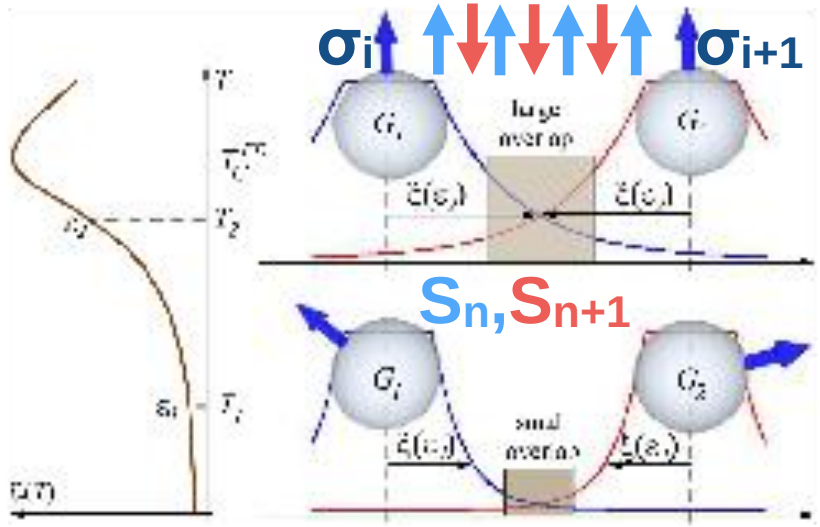
Ferromagnetic nanodots embedded in *TTF-QCl$_4$* thin films

Next: **B9**



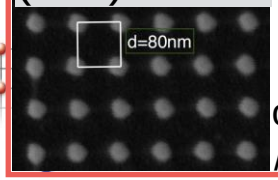
$$\mathcal{H} = J\sum_n [1+(-1)^n\delta]\vec{S}_n \cdot \vec{S}_{n+1}$$

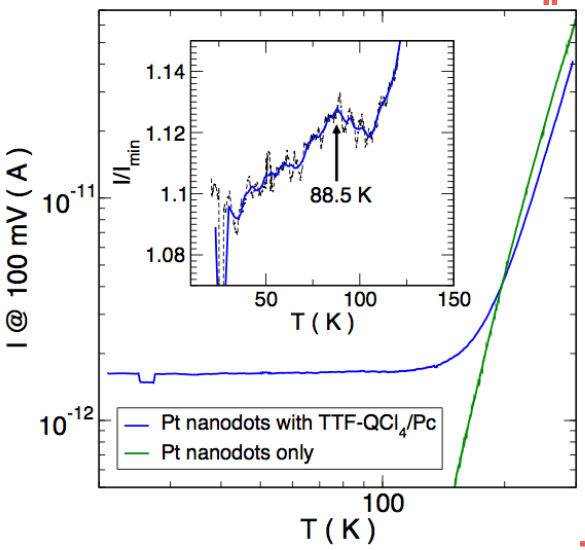
$$\mathcal{H} = J\sum_n [1+(-1)^n\delta]\vec{S}_n \cdot \vec{S}_{n+1}$$

additional coupling to FM grains $+\sum_{n,i} |J'|\vec{S}_n \cdot \vec{\sigma}_i$

First reference measurements
- Pt nanodots
- D≈10nm
- d = 30nm

Co nanodots (test)



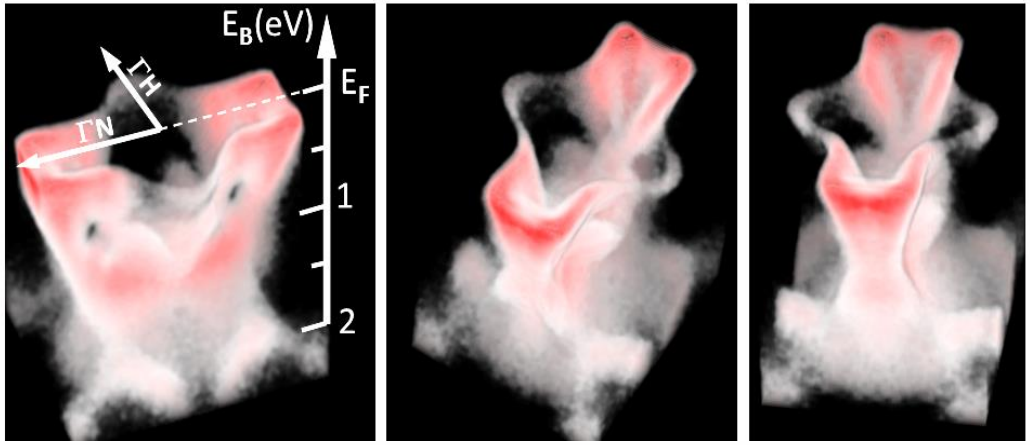


Completion strain-effect study
Conductivity fluctuations (→B11)
New heterostructures
- Exchange-bias-induced spin state pinning at TTF-QCl$_4$/FM interface: ordered AFM state in dimerized spin chain?
- Influence of TTF-QCl$_4$ polarization state on magnetic tunnel exchange coupling of FM nanodots?

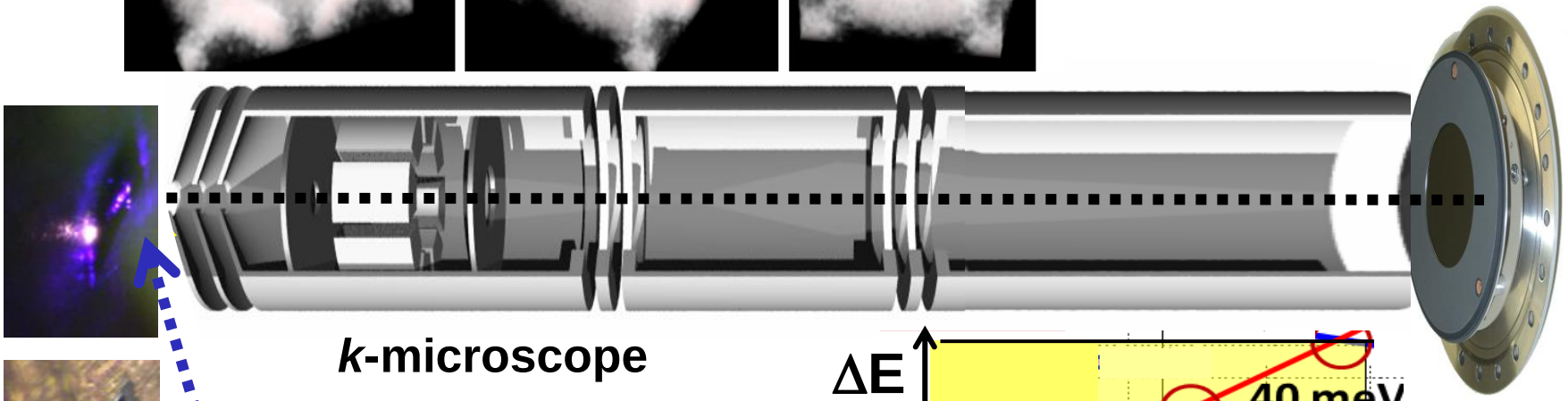
High-Resolution **Photoelectron *k*-Microscopy** of Organic Charge-Transfer Salts at Variable Temperature

Next:

B8



“3D *k*-space object”
Mo(110) surf. res.

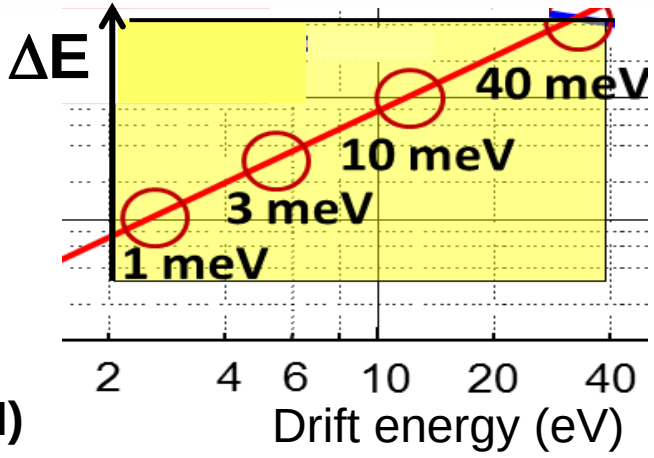


***k*-microscope**

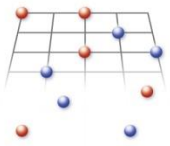
DLD

***κ*-Br**

Ti-sapphire laser



Planned: Sy radiation (BESSY, PETRA III, FLASH)



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Ultramicroscopy, subm. (2014)