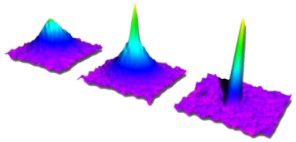
Engineering and controlling quantum matter

Model systems

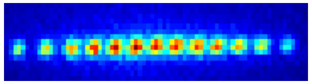
Theoretical ↕ **modelling**

Real materials

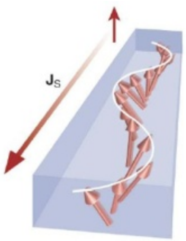
Ultracold quantum gases



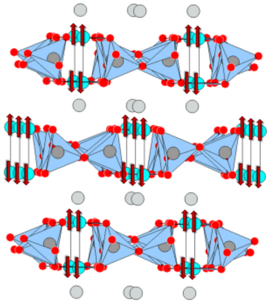
Trapped ions



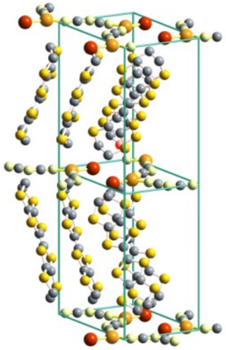
Magnons



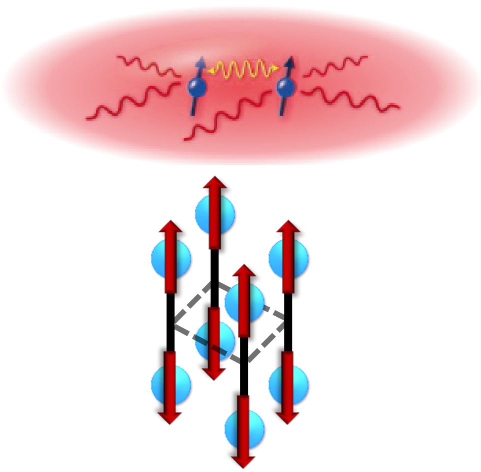
Bulk quantum magnets

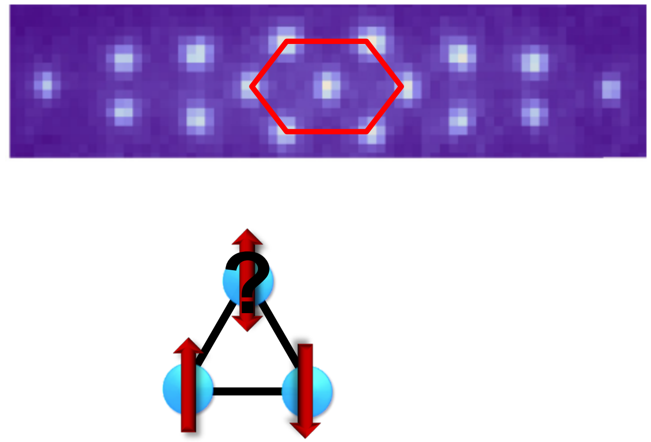


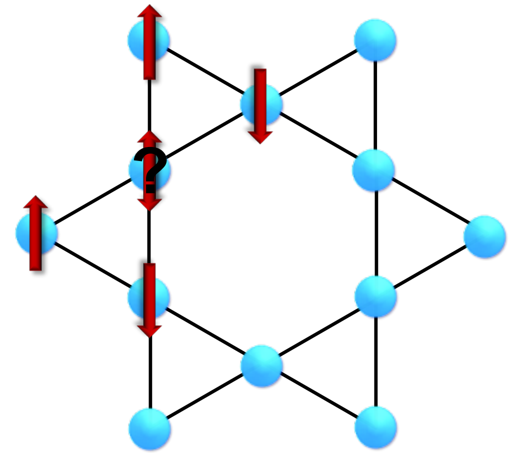
Charge-transfer salts



Real materials as model systems







Coupled dimers

- Bose-Einstein condensation
- Berezinskii-Kosterlitz-Thouless

Triangular lattice

- Spin liquid
- Bose-Einstein condensation

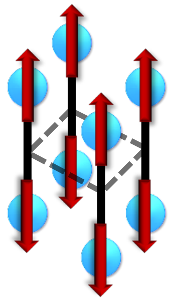
Kagome lattice

- Spin liquid
- Correlated Dirac metal

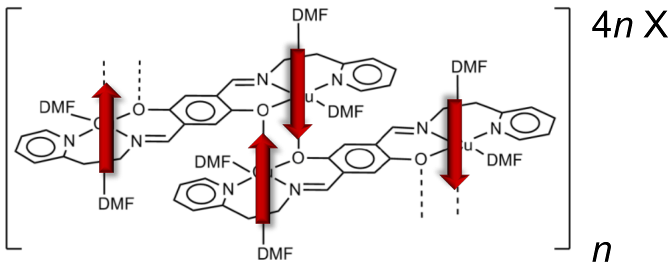
Rational design and tuning by structural and/or chemical modification

Varying dimensionality and frustration

Bulk quantum magnets: Coupled dimers



Cu(II)-p-hydroquinonate coord. polymer

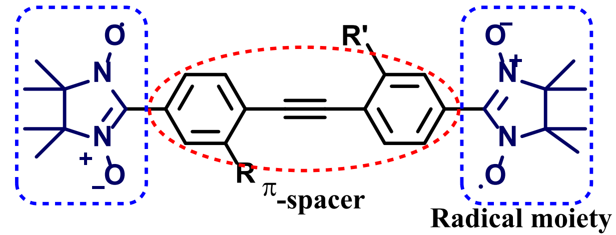


X = $CF_3SO_3^-$

- Cu-based molecules as building blocks
- ***Dimensionality:*** 2D coupled

Nature Commun. **5**, 5169 (2014)

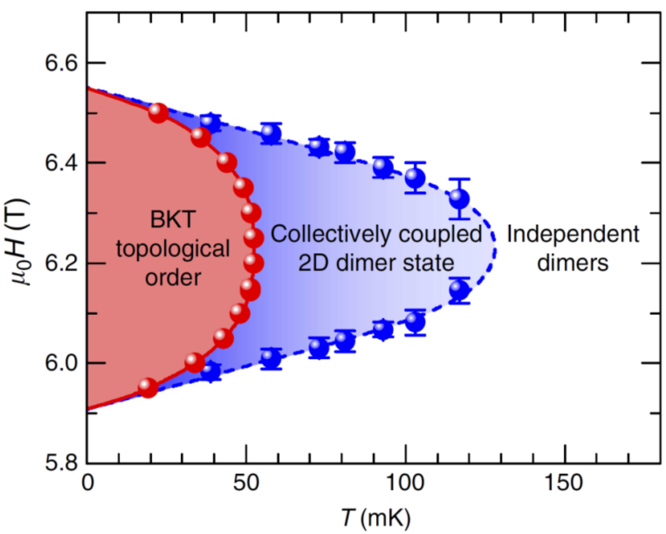
Nitronyl nitroxides biradicals



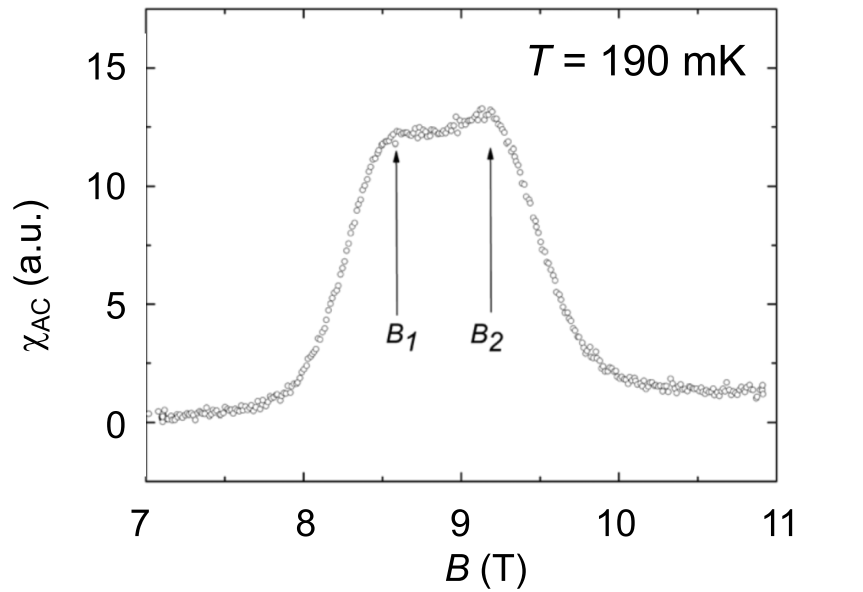
B5

- Organic molecules as building blocks
- ***Tuning parameter:*** π-spacer

Cryst. Growth Des. **12**, 54 (2012); **14**, 5810 (2014)
J. Mater. Chem. C **2**, 6618 (2014)

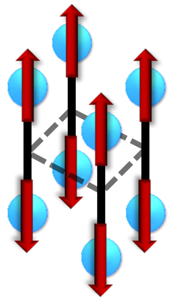


B1
B2
B3
A8



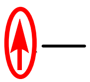
Transregio 49
Frankfurt / Kaiserslautern / Mainz

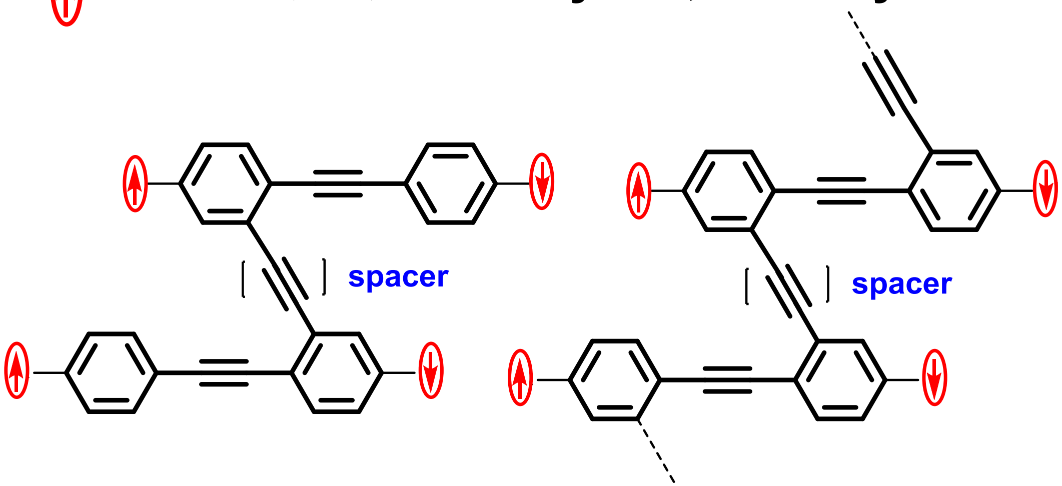
Bulk quantum magnets: Coupled dimers



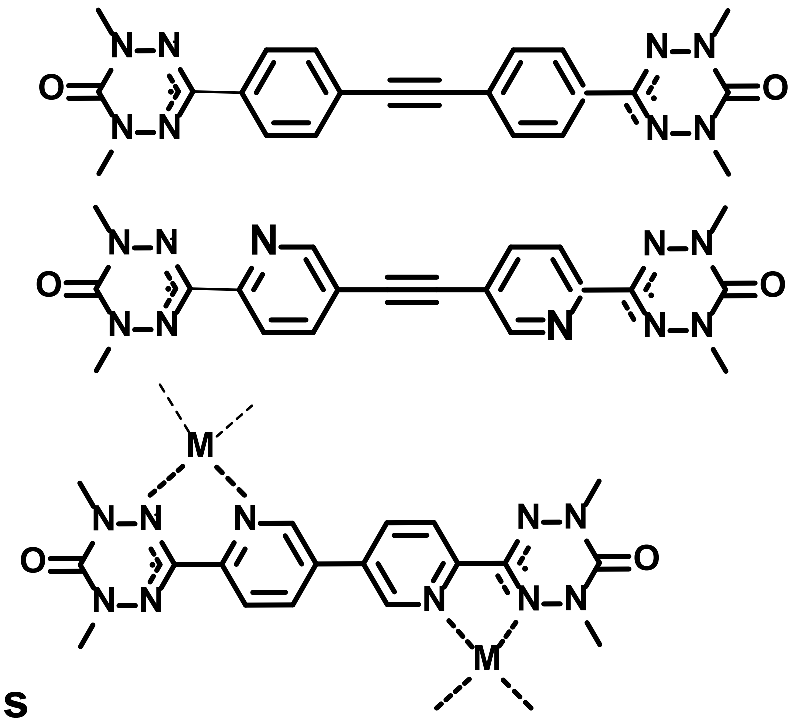
Next:

Covalently linked biradicals

 **= NN, IN, tert-butylNO, verdazyl**



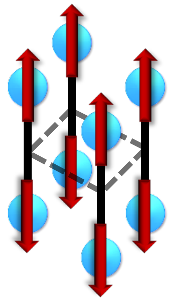
Verdazyls with additional ligation site

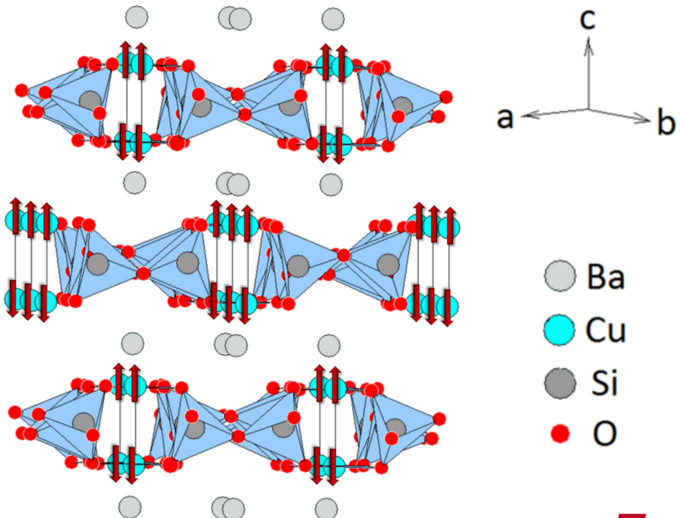


Additional approach: Acceptor based biradicals

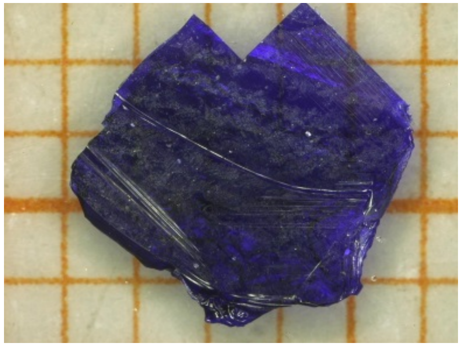
B5

Bulk quantum magnets: Coupled dimers

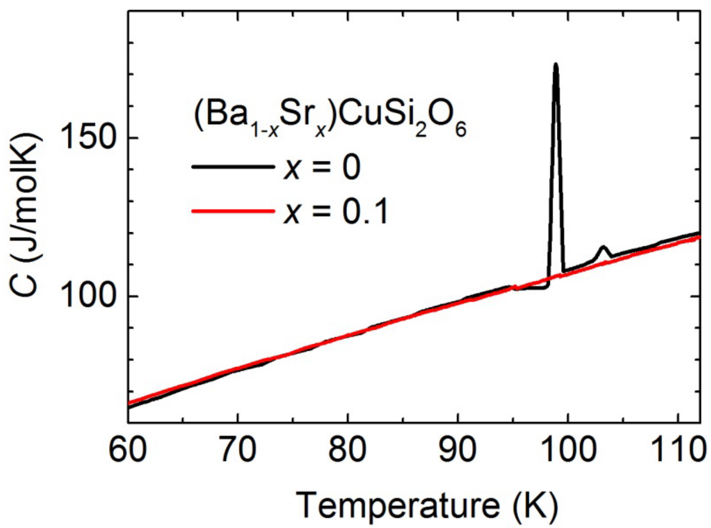




B4



$(Ba_{1-x}Sr_x)CuSi_2O_6$ – Han Purple

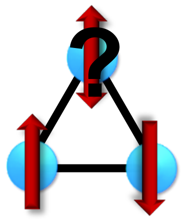


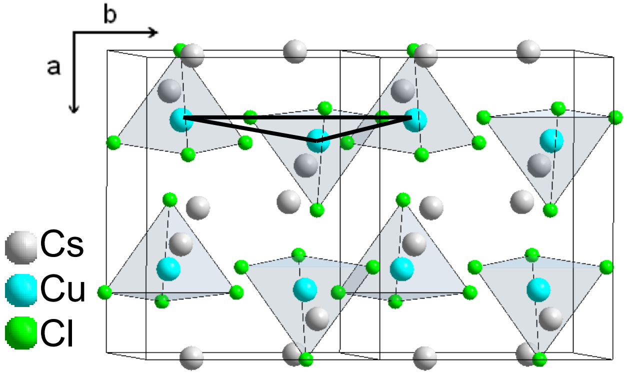
- ***Tuning parameter:*** Sr substitution
- ***Dimensionality:*** Crossover from 3D to 2D accessible

Next:

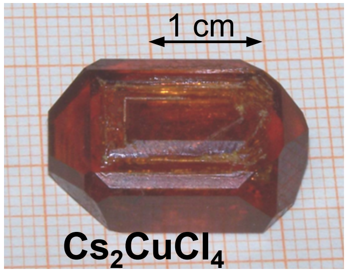
- Crystal growth optimization for x = 0.1 **B4**
- Detailed low-temperature characterization **B1**
- Calculation of coupling constants **$B13_N$**

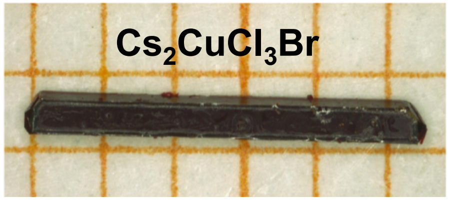
Bulk quantum magnets: 2D-triangular lattice

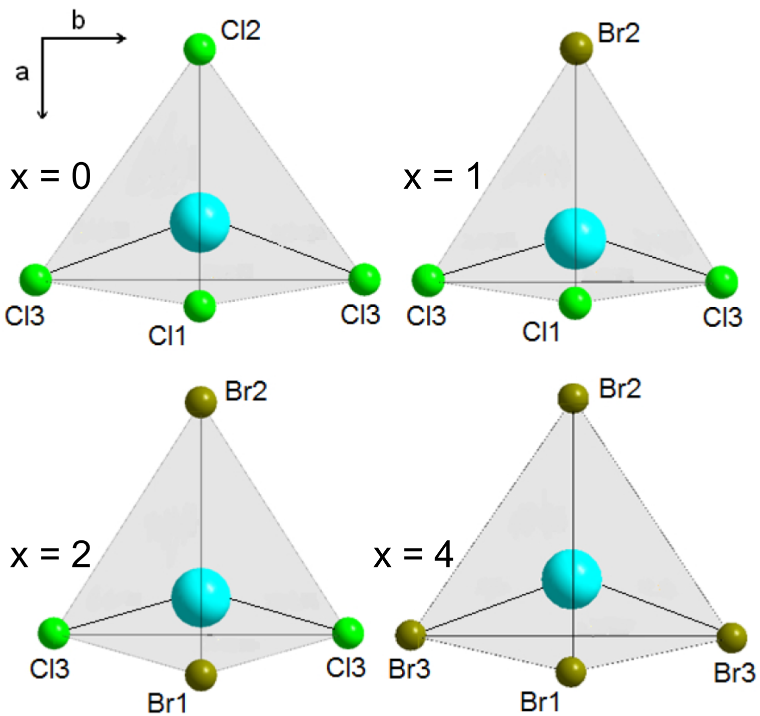




B4







- **$Cs_2CuCl_{4-x}Br_x$:** Large single crystals available
- ***Tuning parameter:*** A8

  Magnetic field and Br-content x B1

  Phys. Rev. B **91**, 041108(R) (2015) B2

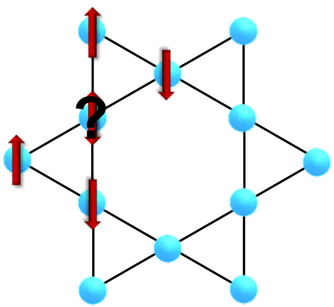
  Phys. Rev. B **91**, 035124 (2015)

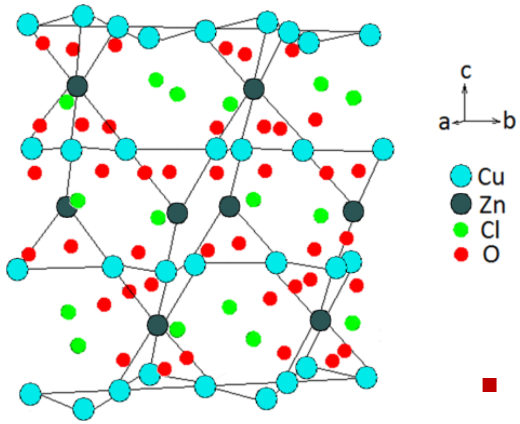
Next: Focus on crystals with x = 1 and 2

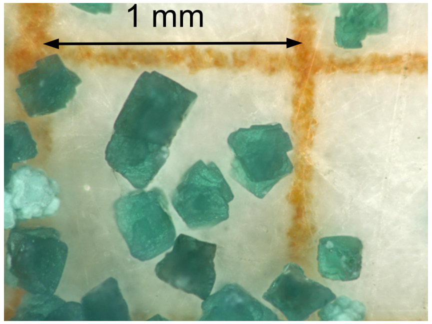
- Magnetic ground state B1
- Field induced QCP A8
- Coupling constants $B13_N$

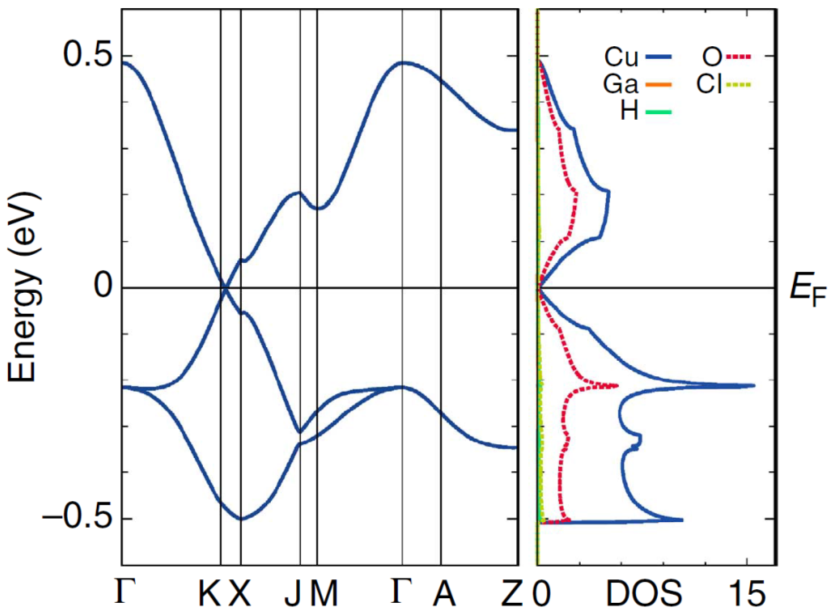
Transregio 49
Frankfurt / Kaiserslautern / Mainz

Bulk quantum magnets: 2D-Kagome lattice









- **$ZnCu_3(OH)_6Cl_2$**: Hydrothermal synthesis **B4**
- DFT calculations: $GaCu_3(OH)_6Cl_2$ (n=4/3) Dirac point at E_F
- Proposal of a correlated Dirac metal **B2**

Phys. Rev. B **88**, 075106 (2013)

Nature Commun. **5**, 4261 (2014)

Next:

- Synthesis of substituted samples **B4**
- Many variants possible: $ACu_3(OH)_6(FBr)$ **B1**
- Tunable by charge doping: Ga^{3+} on Zn^{2+} **B2**
- Kagome lattice at incommensurate filling **B3**

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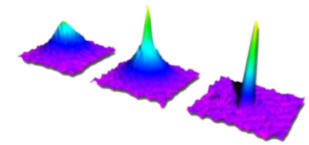
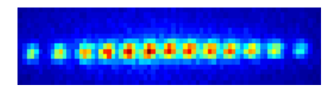
Theoretical ⇕ **modelling**

Real materials

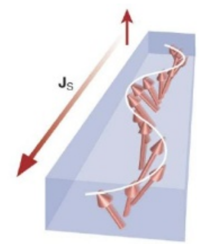
Ultracold quantum gases



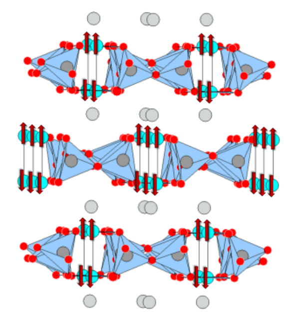
Trapped ions



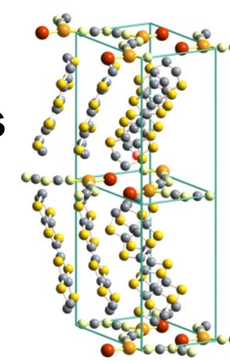
Magnons



Bulk quantum magnets

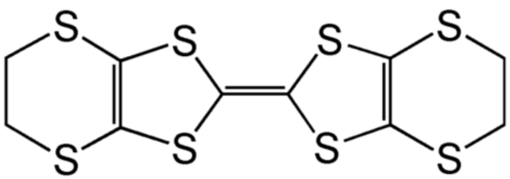


Charge-transfer salts

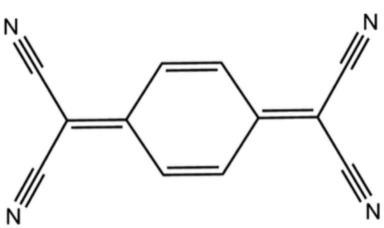


Charge-transfer salts

Charge-transfer complexes from organic building blocks can adopt different columnar structures

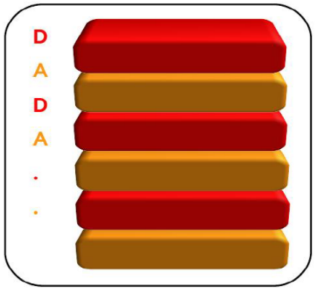


Donor: BEDT-TTF (ET)

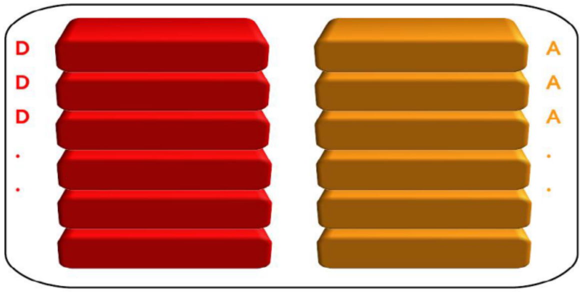


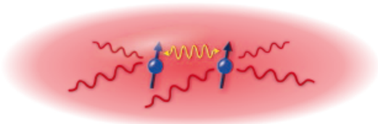
Acceptor: TCNQ

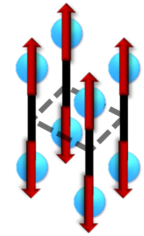
Donor/Acceptor

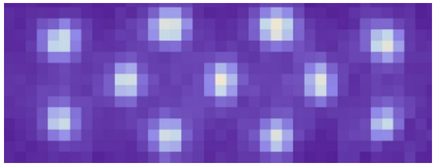


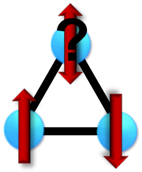
Donor **Acceptor**



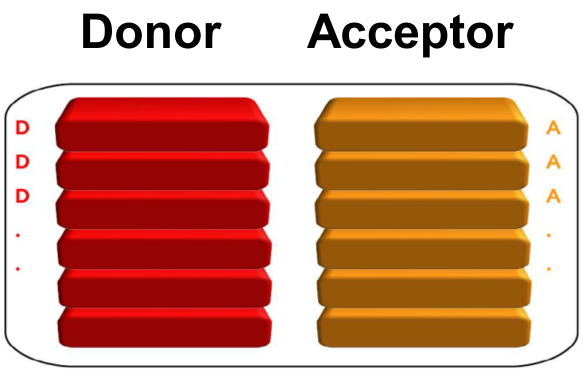


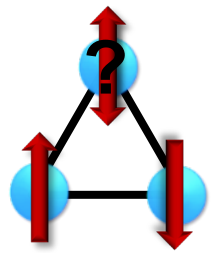


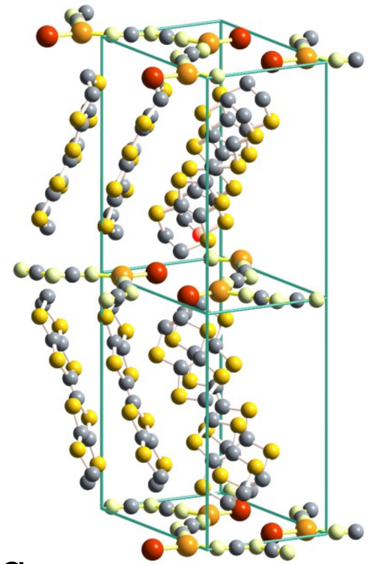


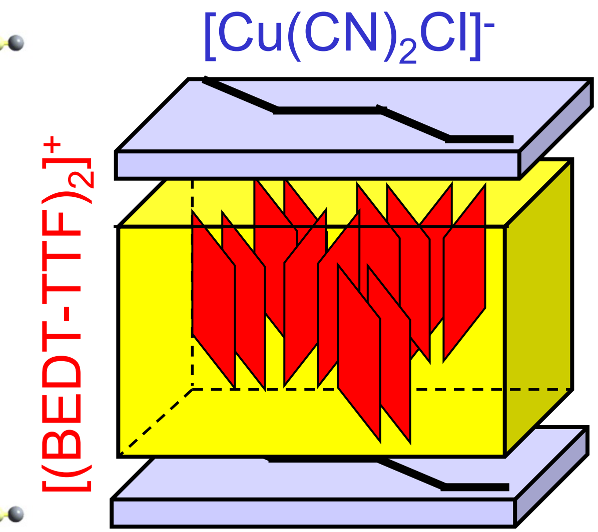


Charge-transfer salts: Segregated stacks







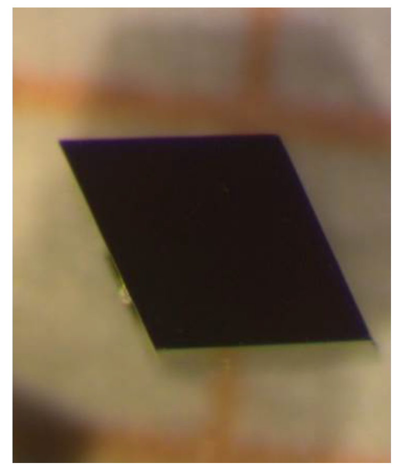


B6

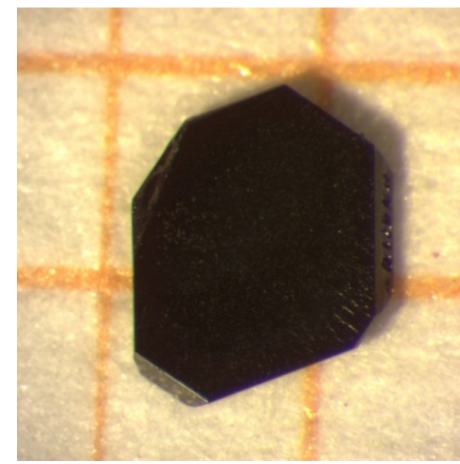
- Successful single crystal growth
- Tunable by pressure, composition, cooling
- κ-$(ET)_2Cu[N(CN)_2]Cl$: First multiferroic charge transfer salt

  Nature Materials **11**, 755 (2012)

B6 **B11**



κ-$(ET)_2Cu[N(CN)_2]Cl$

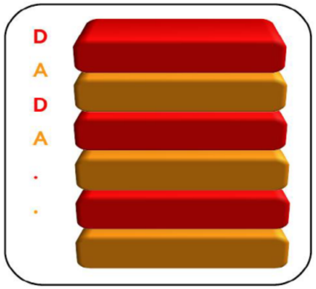


κ-$(ET)_2Hg(SCN)_2Cl$

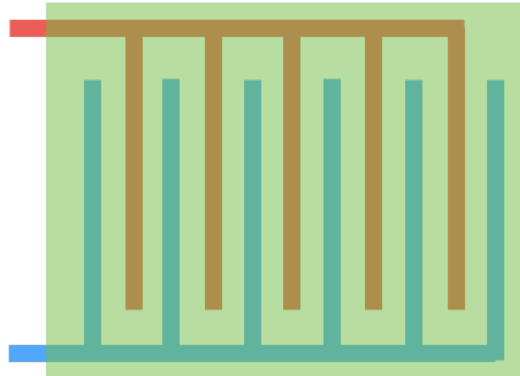
Next: Detailed study of unusual metal-insulator transition in κ-$(ET)_2Hg(SCN)_2Cl$

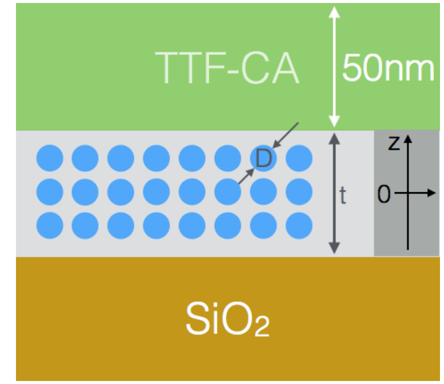
Charge-transfer salts: Mixed stacks

Alternating Donor/Acceptor



B9



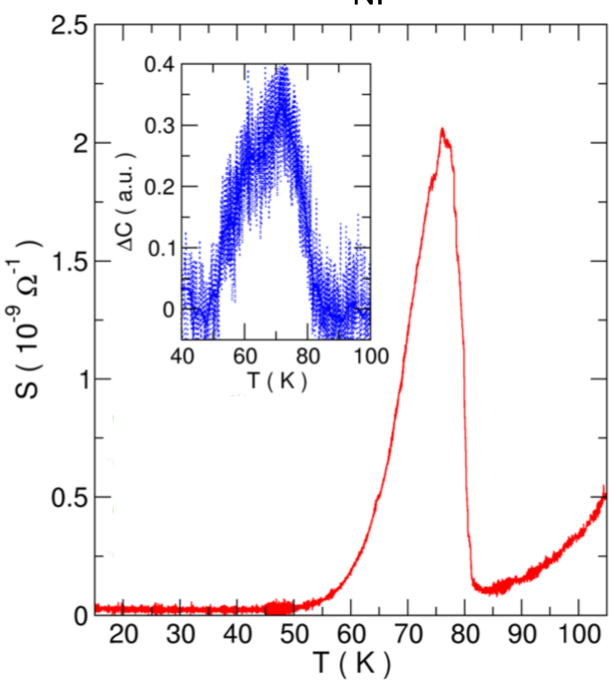


- Dimerization of acceptor-donor molecules in TTF-CA
- Ferroelectric ground state below neutral-ionic (NI) trans.

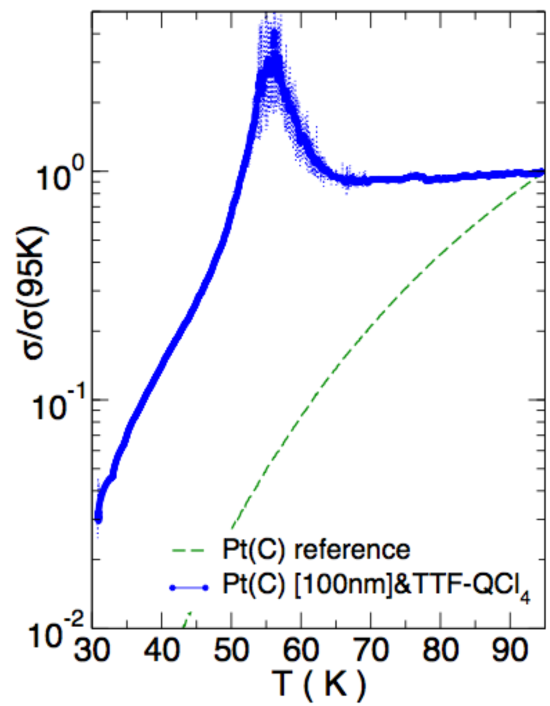
Mater. Res. Expr. **1**, 046303 (2014)

Next:
- Tuning of the NI transition
- Utilizing strain effects

TTF-CA 5 µm film
Bulk-like T_{NI} = 81 K

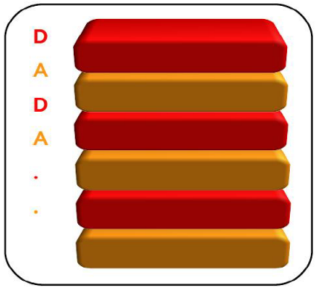


TTF-CA 50 nm film
Reduced T_{NI} = 56 K



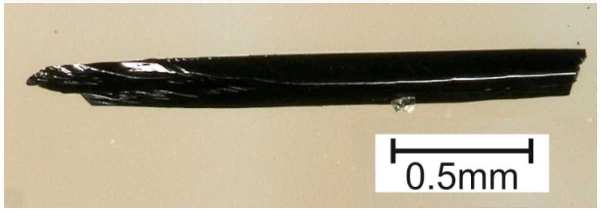
Charge-transfer salts: Mixed stacks

Alternating Donor/Acceptor

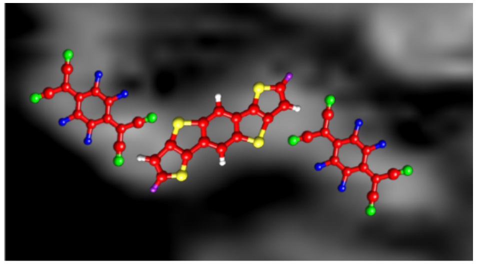


DTBDT-F_4TCNQ

Single crystal



Thin film



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

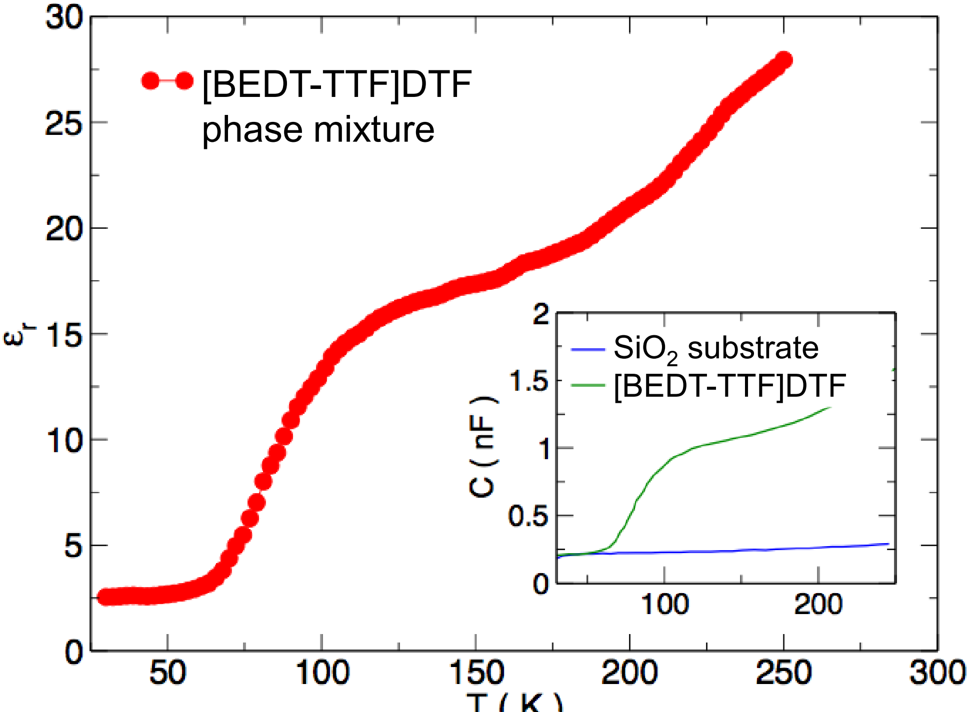
- Several new CT salts prepared, e.g. TMP/HMP-TCNQ, DTBDT-F_4TCNQ
- Both as thin films and single crystals

J. Am. Chem. Soc. **134**, 4699 (2012)

Phys. Rev. B **89**, 075435 (2014)

Next:

- [BEDT-TTF]DTF: New system with possible neutral-ionic transition



B9

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Theoretical ↕ **modelling**

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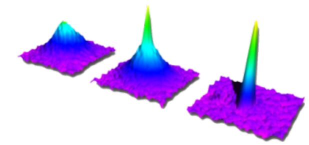
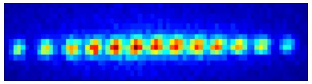
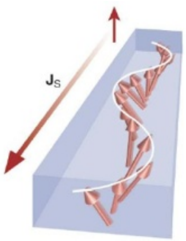
Ultracold quantum gases



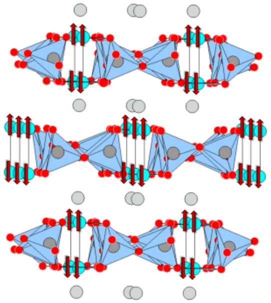
Trapped ions



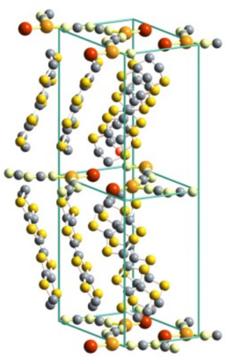
Magnons



Bulk quantum magnets



Charge-transfer salts



Materials Design – Synthesis & Modelling

	Frankfurt am Main	Kaiserslautern	Mainz
Materials Design - Synthesis & Modelling	B1, B2, B4, B6, B13N	A7, A9, A12	A10, B5, B8
Cooperative Phenomena	A3, A8, B1, B2, B4, B6, B9, B11, B13N	A5, A7, A9, A12, B3	A10, B5, B8, B12
Excitations & Interactions	A3, A8, B1, B2, B4, B6, B9, B11, B13N	A5, A7, A9, A12, B3	A10, B5, B8, B12