

B1

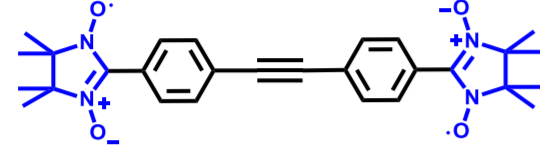
Interacting magnetic excitations in quantum spin systems - Thermodynamic investigations

Bernd Wolf, Michael Lang (Universität Frankfurt)

New materials with extended range of field-induced "order"

B1 B2 B3 B5

- promising candidate tolan-bridged biradical: nitronyl nitroxide (synthesis in B5)



- MEAM 154: $J_{\text{intra}}/k_B \sim 10$ K
- field-induced "ordered phase" is extended by a factor of nearly 4 (in temperature)

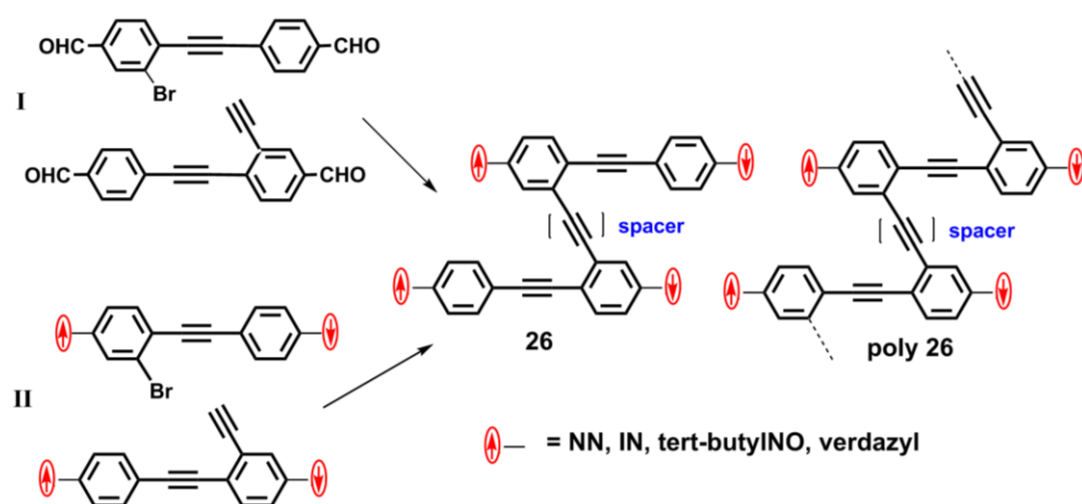
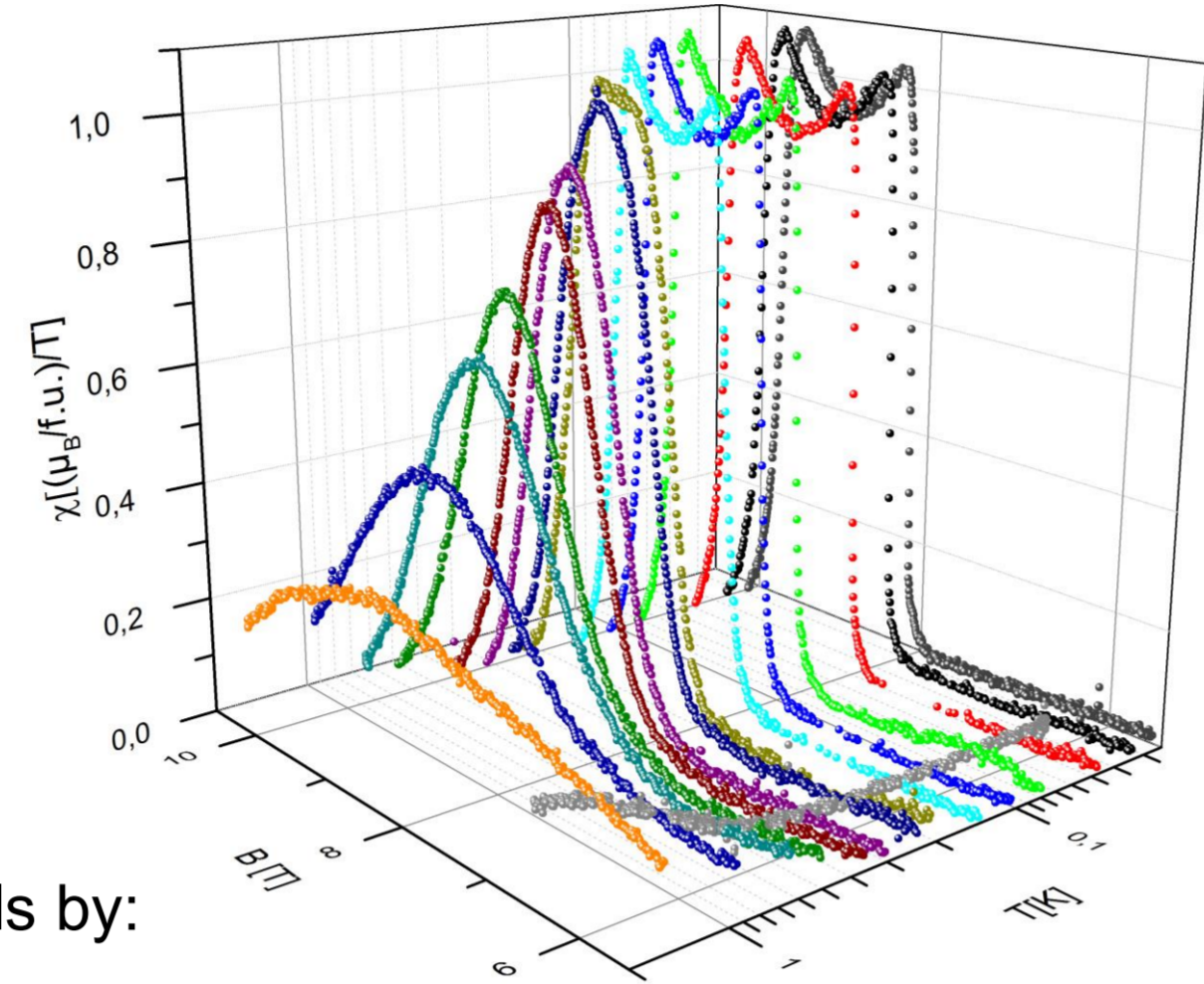
- $\chi(T, B)$ striking similarity to TK 91

- preliminary QMC simulations in B3

Goals and work programme

- characterization of field-induced "order" in biradicals by:
 - specific heat
 - if large single crystals are available: elastic constants and thermal expansion

- dimer-systems with different inter-dimer interactions by using modified bridging units such as CONH₂, OMe, NO₂ or Br

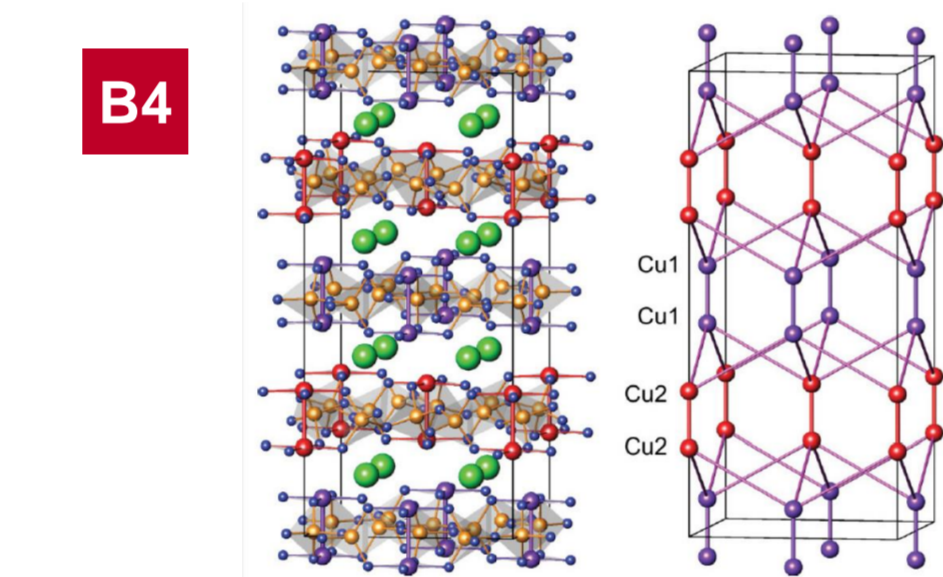
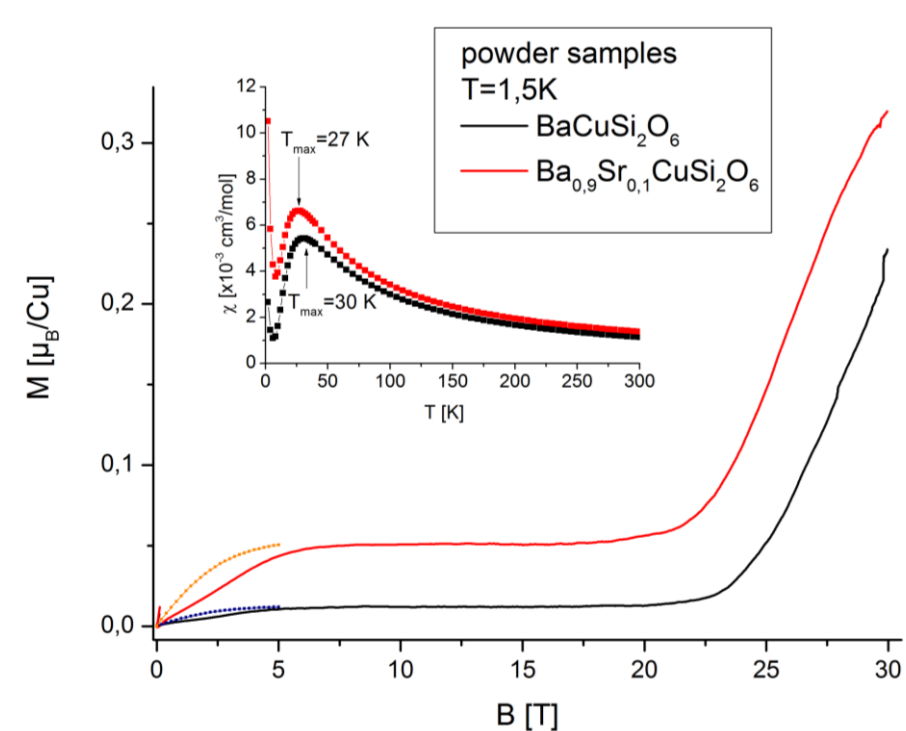


- metalorganic coupled-dimer systems: modified (Ba,Sr)Cu₂Si₂O₆

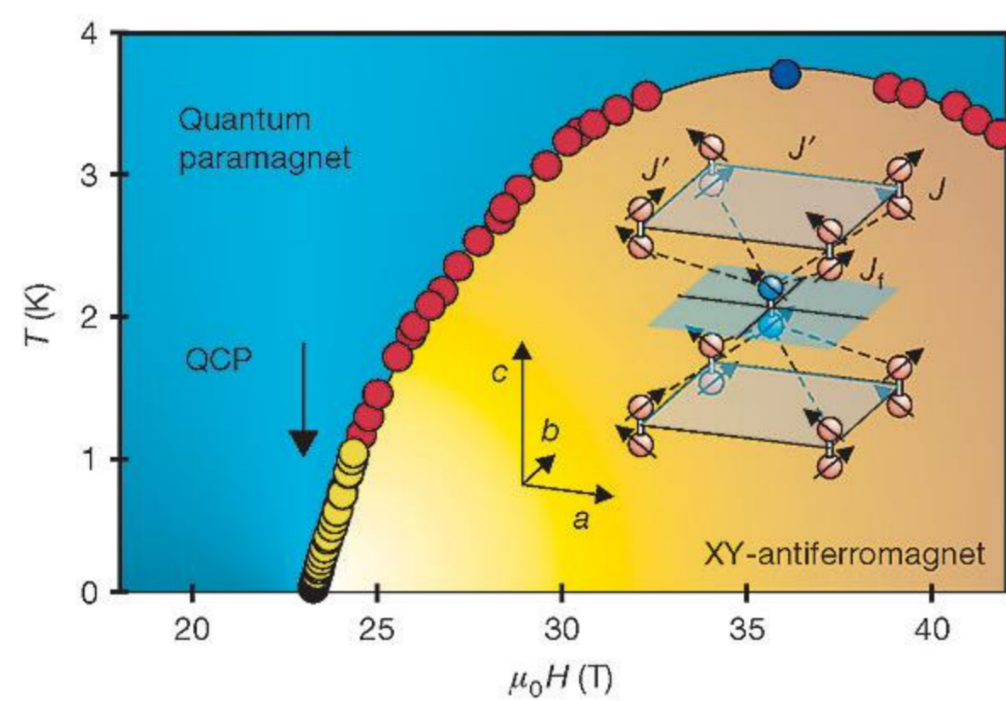
- influence of the structural transition on the field-induced ordering?

- Suppression of the structural transition at $T \approx 100$ K by Sr doping
 - study the influence on the field-induced "ordering"

- theoretical support from B2 B3 B13N



D. V. Shepyakov et al., PRB 86, 014433 (2012)



Sebastian et al., Nature 441, 617

- preliminary results on $\chi(T)$ and $M(B)$

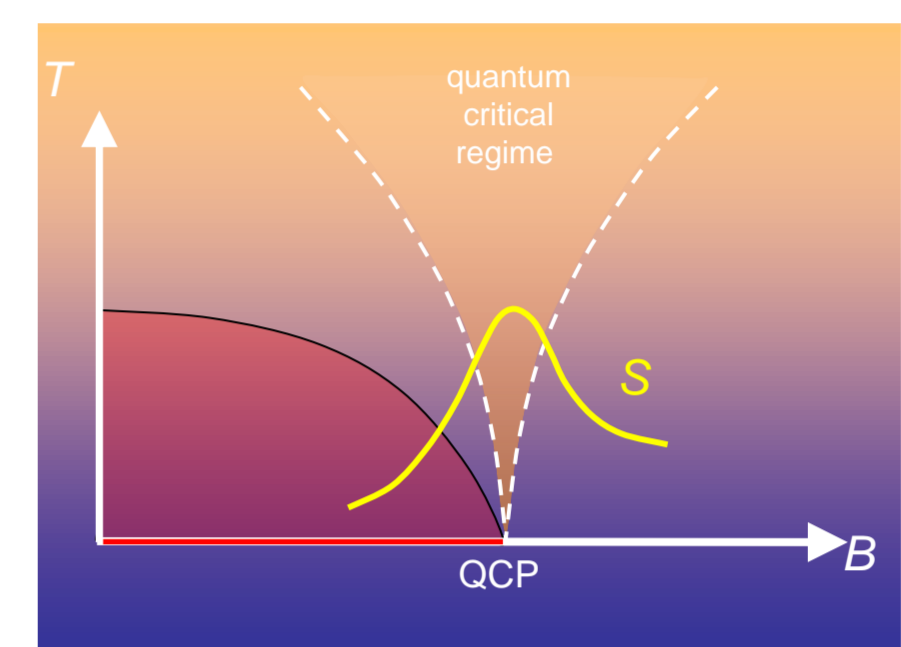
iii) Studying the critically enhanced magnetocaloric effect near a B-induced quantum-critical point

Achievements

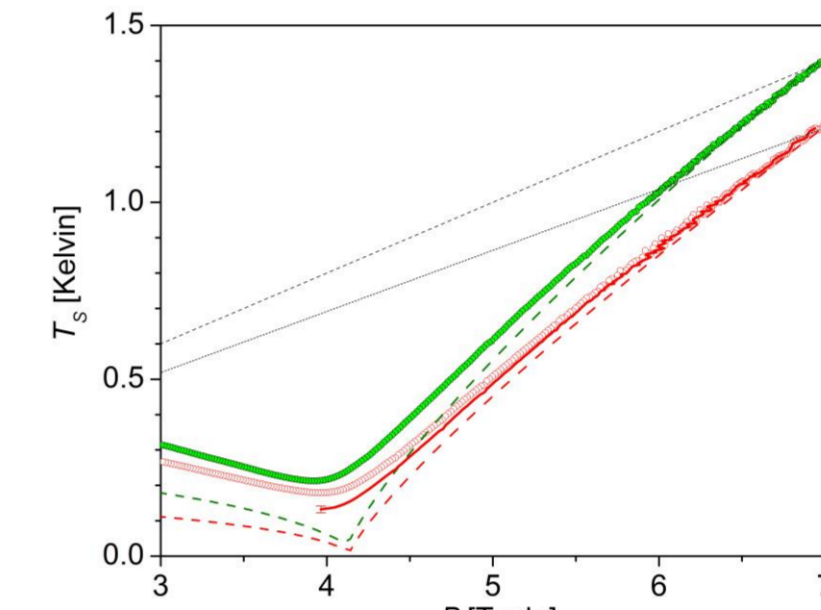
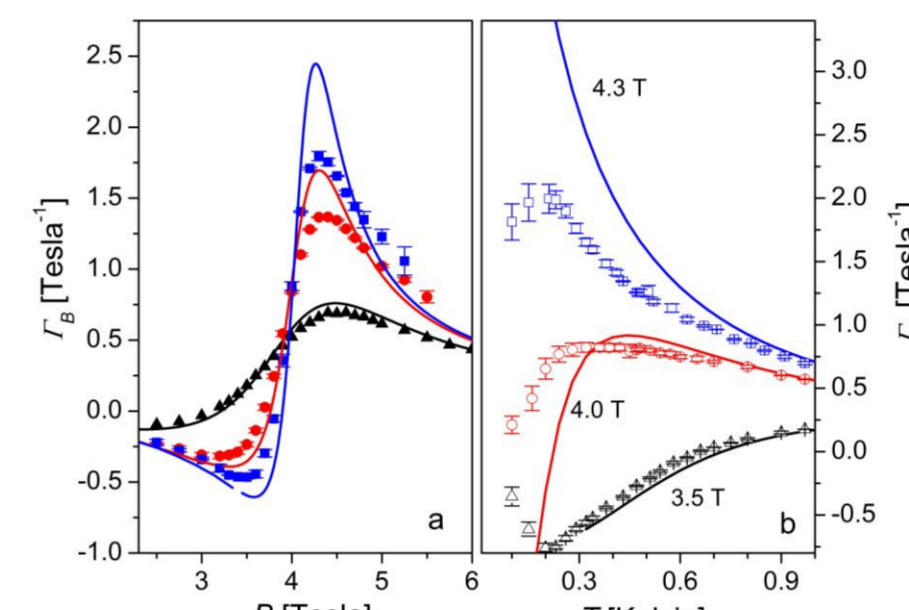
Novel interaction-driven cooling processes in ultra cold quantum gases and solid state systems:

solid state systems:

- the accumulation of entropy around a magnetic field-induced quantum-critical point (QCP)
 - enhanced magnetocaloric effect (MCE) expected



- proof of principle on an afm Heisenberg S = 1/2 chain (AFHC): a simple quantum-critical system



A3 B1

Joint publication:

Wolf et al., Int. J. Mod. Phys. B 28, 1430017 (2014)

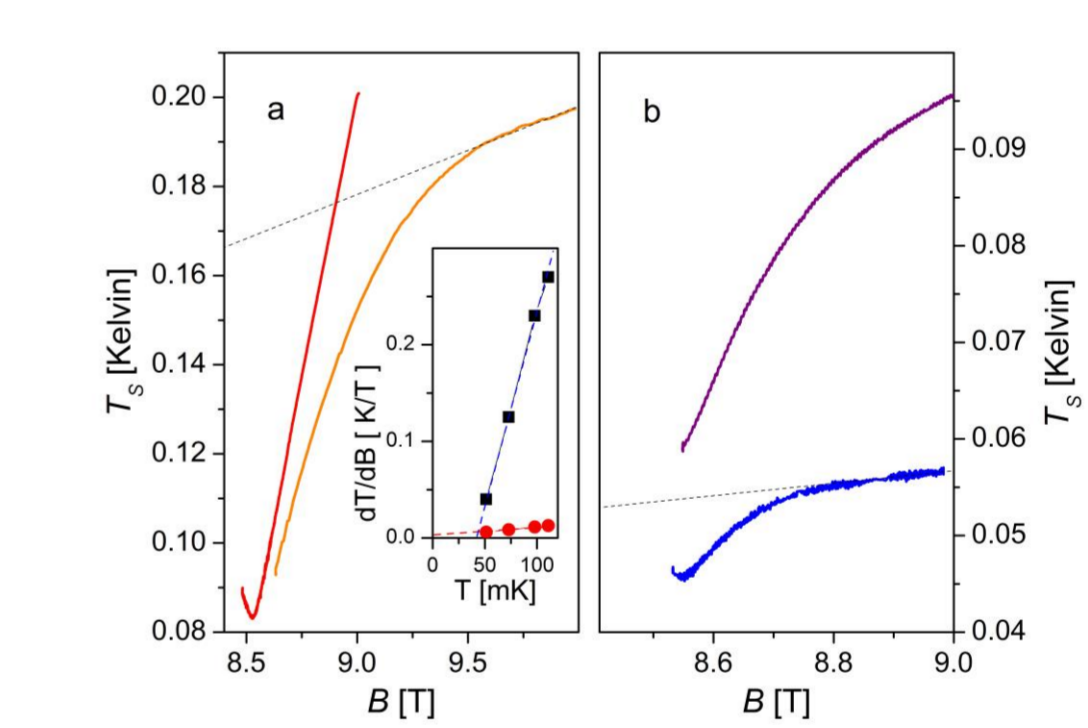
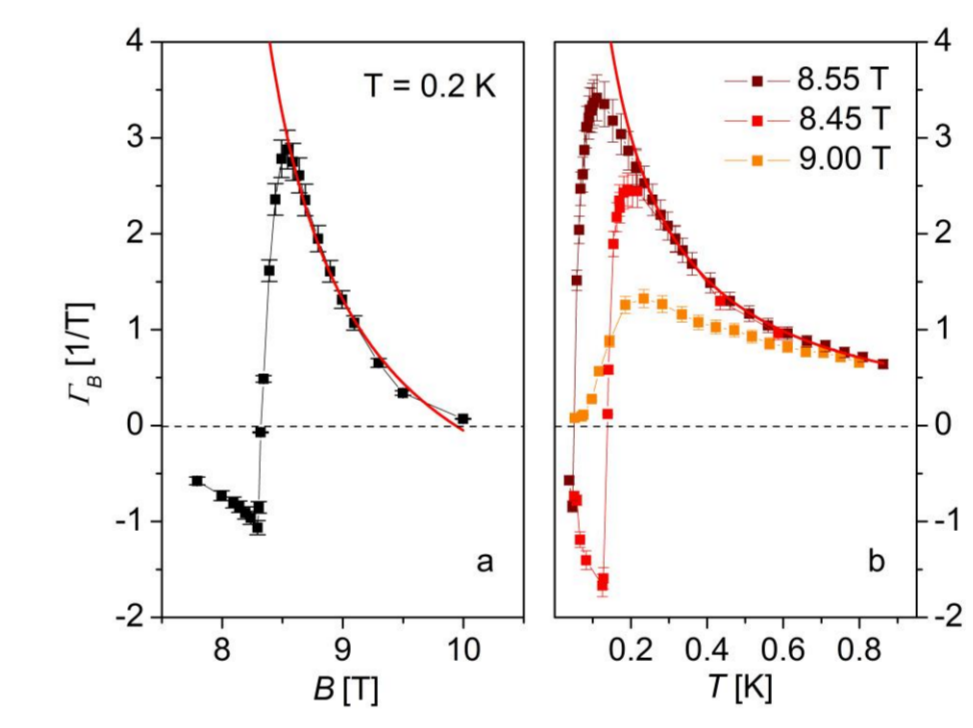
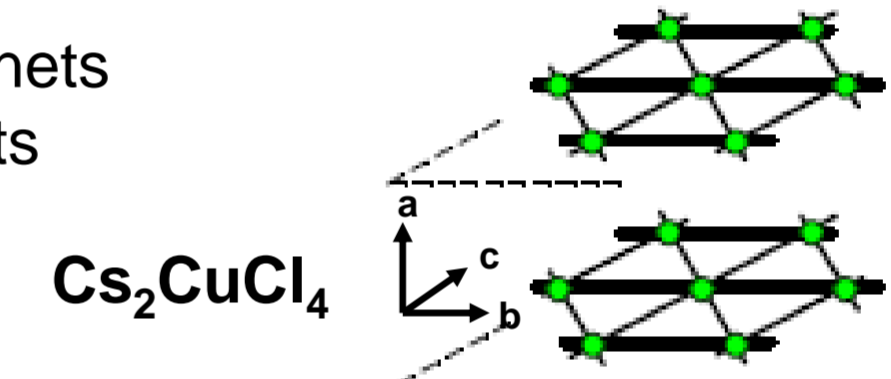
Wolf et al., Proc. Natl. Acad. Sci. USA 108, 6862 (2011)

- diverging Grüneisen and sign change at the QCP

- superlinear cooling curves

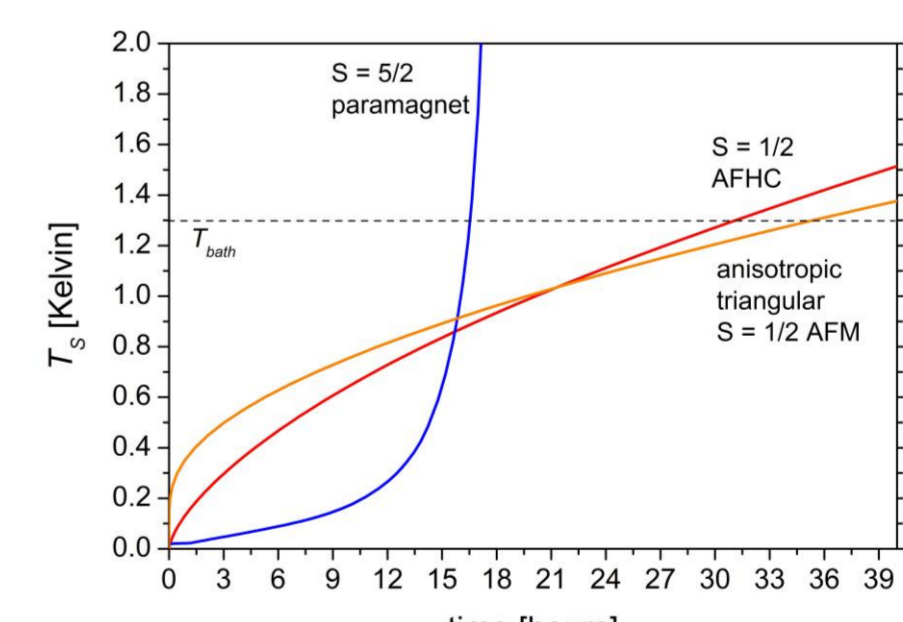
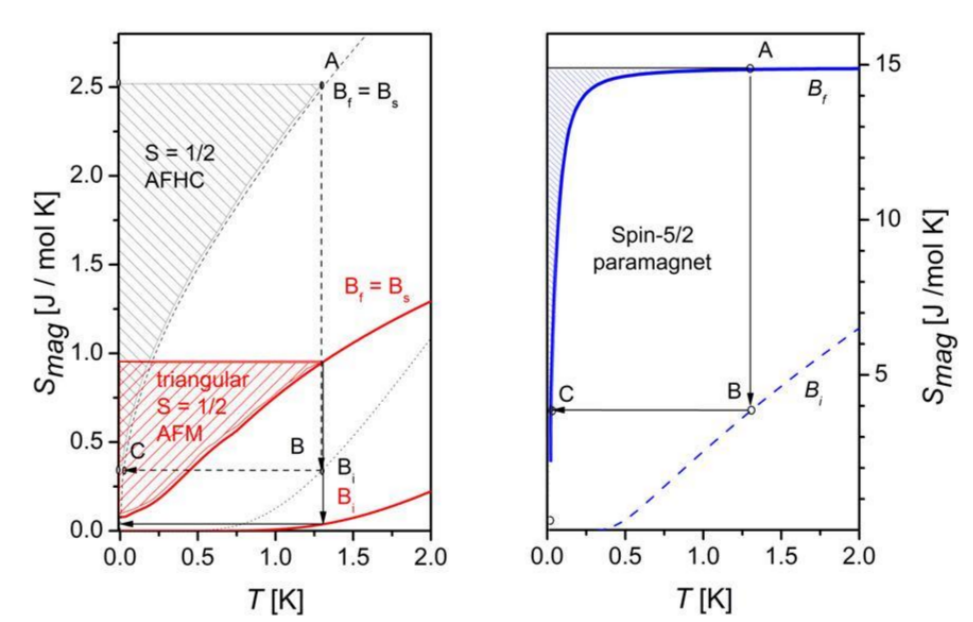
- extension: frustrated quantum magnets
 - 2D triangular antiferromagnets

Lang et al., Phys. Status Solidi B 250, 457 (2013)



- efficiency: $\Delta Q_c / \Delta Q_m$

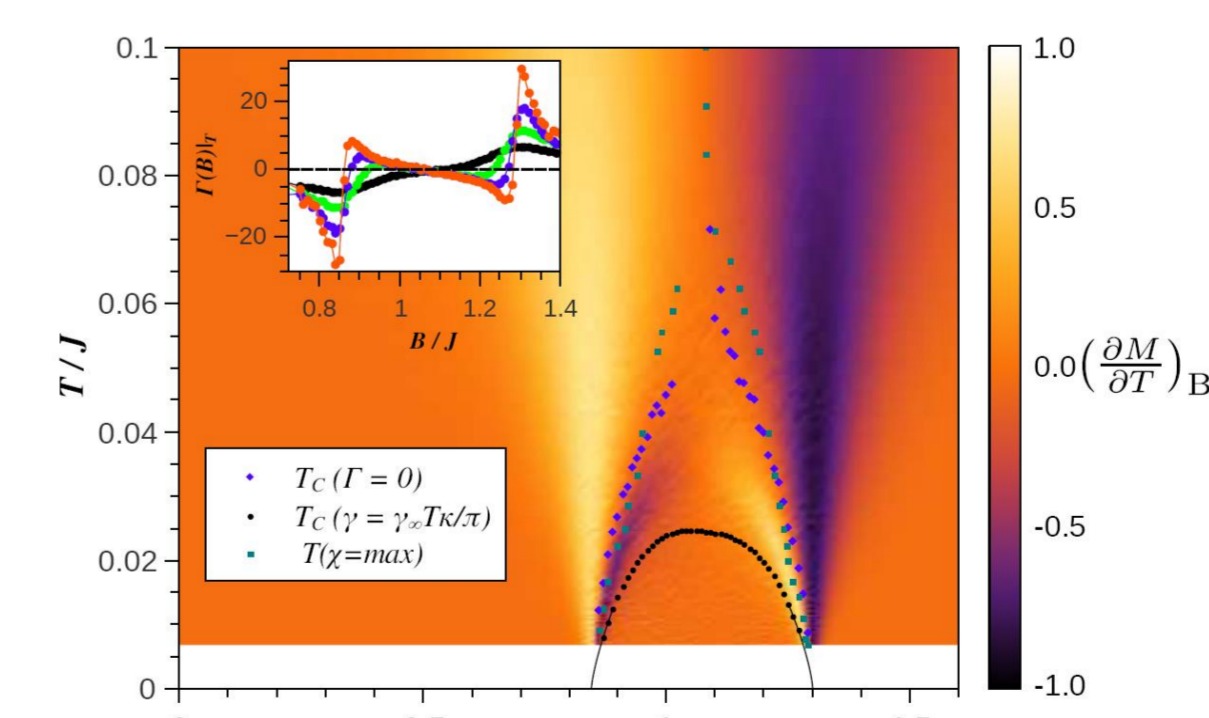
$$\Delta Q_c = \int_{T_i}^{T_f} T \cdot \left(\frac{\partial S}{\partial T} \right)_B dT \quad \Delta Q_m: \text{rectangle AB} \times \text{BC}$$



for applications:
sample temperature as a function of time for
- 100 cm³ material
- 5 μW heat load

paramagnet: ~10%; AFHC: ~25%; 2d triangular afm: ~50% !!

Goals and work programme



- MCE in strongly frustrated triangular AFMs
 - determination of $\Gamma_B(T, B)$ (e.g. Cs₂CuCl₂Br₂)
 - identification of QCPs
 - investigating the cooling performance of the novel mixed systems

B4

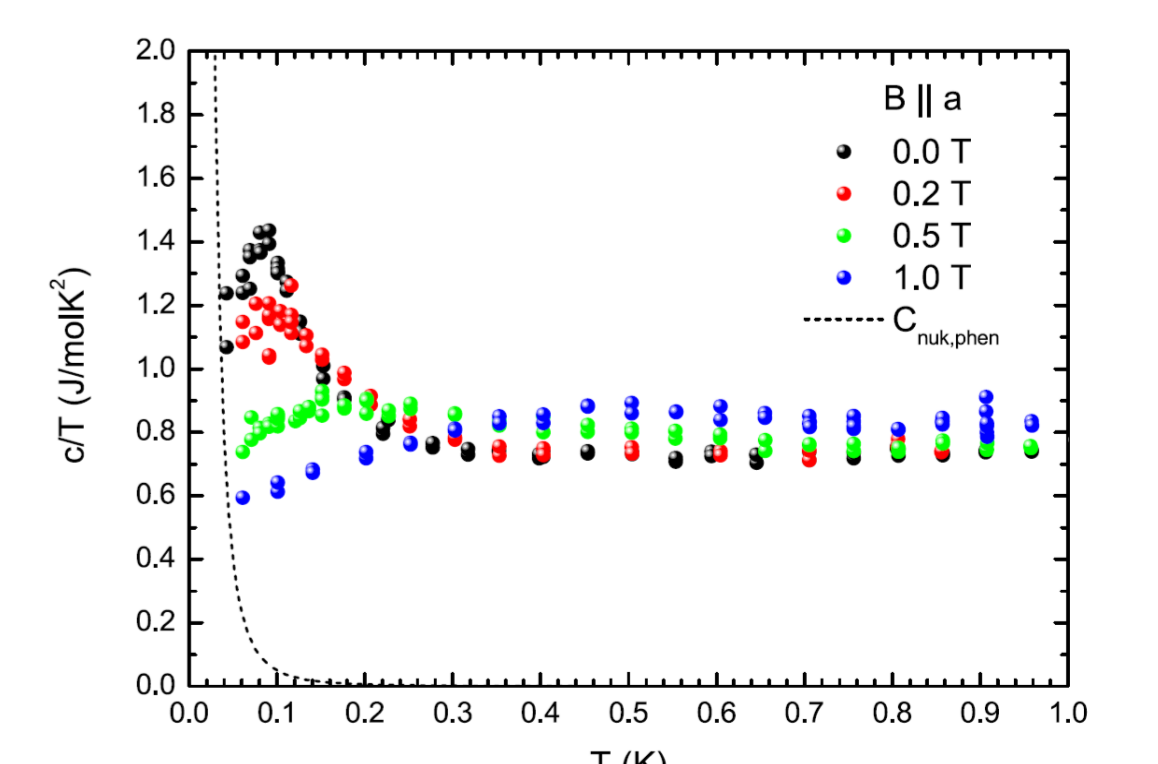
MCE in coupled-dimer systems

- measurements performed on stable organic biradicals (e.g. MEAM154)

- theoretical support

A8 B3

Straßel et al., arXiv, 1412.0266v1 (2014)



Requested staff

Dr. Oleksandr Foyevtsov (Postdoc)

- thermal expansion and magnetostriction on spin-liquid-candidate systems such as the novel kagome-lattice systems, selected members of the Cs₂CuCl_{4-x}Br_x, spin-liquid candidates of the charge-transfer salts (B6)
- low-temperature ultrasonic measurements around their B-induced QCPs effects of spin-lattice interactions on the quantum-critical properties

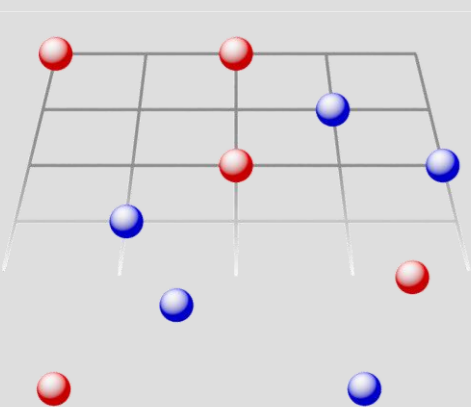
Lars Postulka (Ph.D. Student)

- high-resolution susceptibility measurements on the field-induced ordered states
- development of a phase-sensitive detection technique for $\chi(T, B)$ in pulsed magnetic fields

Role within the SFB/TR 49

Close collaborations exist to the following projects

- B2 \Rightarrow *ab initio* DFT- calculations for magnetic coupling constants
- B3 \Rightarrow Quantum Monte Carlo simulations / analytical calculations for coupled spin-dimer systems
- B13N \Rightarrow *ab initio* QMC for coupling constants; perturbation approach for spin phonon interaction
- B4 B5 \Rightarrow characterization of the various materials; feedback to the synthesis
- A8 \Rightarrow microscopic model including spin-phonon interactions for addressing the elastic behaviour (ultrasonic attenuation and elastic constant) around the QCPs
- A3 \Rightarrow further extending the concept of "cooling through many-body interactions" to quantum gases



Transregional Collaborative Research Centre SFB/TR 49
Frankfurt / Kaiserslautern / Mainz