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Mott physics and quantum phase transitions in molecular solids

Solids, made up of molecular units containing open shell transition metal ions or stable organic π -radicals, provide flexible systems for exploring correlated electrons and spins under well-controlled conditions. In the course of an interdisciplinary research program performed within the SFB/TR 49, Frankfurt-Kaiserslautern-Mainz, a variety of molecule-based materials has been synthesized and investigated in detail.

One focus of the investigations lies on the quasi-twodimensional molecular metals of the κ -(BEDT-TTF)₂X family, where transitions between various states such as Mott-insulating, anomalous metallic and superconducting can be induced by small variations of chemical (substitution) or physical (pressure, temperature) parameters. The ability to fine-tune the materials' electronic parameters, i.e., the strength of the on-site Coulomb repulsion relative to the band width, enables one to explore fundamental aspects of strongly correlated electrons in reduced dimensions. In this talk I will address the Mott transition in BEDT-TTF-based materials, the question of its criticality [1, 2] and the recently observed multiferroic properties on the insulating side of the transition [3].

A second class of materials is formed by low-dimensional quantum magnets where the molecular components provide a magnetic exchange coupling, weak enough for laboratory magnets to tune the systems close to a field-induced quantum-critical point – a $T = 0$ phase transition. Here I will address the anomalous magnetocaloric effect observed in a Cu²⁺-containing coordination polymer, a very good realization of a spin-1/2 antiferromagnetic Heisenberg chain. In a proof-of-principle demonstration it has been shown that the accumulation of entropy around a quantum phase transition can be used for realizing a very efficient and flexible magnetic cooling [4].

- [1] M. de Souza et al, Phys. Rev. Lett. 99, 037003 (2007)
- [2] L. Bartosch et al., Phys. Rev. Lett. 104, 245701 (2010)
- [3] P. Lunkenheimer et al., Nat. Mater. 11, 755 (2012)
- [4] B. Wolf et al., PNAS 108, 6862 (2011)

2. November 2012, 14:00 Uhr

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