Probing charge- and lattice effects around the (presumably Mott) metal-insulator transition in κ-$(BETS)_2Mn[N(CN)_2]_3$

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The organic conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ (κ-Mn) undergoes a metal-insulator (MI) transition at $T_{MI} \sim 25$ K [1,2] accompanied by an antiferromagnetic order of the π spins [3]. Due to a rather weak π-d coupling [4], the insulating ground state cannot be attributed to the influence of the Mn^{2+}-related magnetic degrees of freedom in the anion sublattice. Instead, Coulomb correlations appear to be the driving force for a Mott insulating state, consistent with the material's *p-T* phase diagram [2] which shares some similarities with those of the κ-$(ET)_2X$ salts.

To investigate the insulating ground state, we have performed a comprehensive study of κ-Mn, including fluctuation (noise)- and dielectric spectroscopy together with thermal expansion measurements. We find a first-order MI phase transition giving rise to a drastic increase in the normalized resistance noise power spectral density, accompanied by spatially correlated fluctuators, and an unexpected current (electric field) dependence of the charge carrier dynamics. We argue that these results suggest electronic ferroelectricity caused by the localization of charge carriers within the dimer, as proposed in a number of dimer-Mott insulators [5,6]. In fact, indications for such a behavior is revealed by measurements of the dielectric constant yielding a frequency-dependent maximum below $T_{MI.}$

References

[1] Kushch et al., J. Am. Chem. Soc. **130**, 23, 7238–7240 (2008).
[2] Zverev *et al*., Physical Review B **82**, 155123 (2010).
[3] Vyaselev *et al*., Crystals **2**(2), 224-235 (2012).
[4] Riedl *et al*., Physical Review Letters **127**, 147204 (2021).
[5] Lunkenheimer *et al*., Nature Materials **11**, 775-758 (2012)
[6] Müller *et al*., Physical Review B **102**, 100103(R) (2020).