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Multiferroics by design with frustrated molecular magnets YOSHITOMO KAMIYA, RIKEN, CRISTIAN BATISTA, University of Tennessee, Knoxville, Oak Ridge National Laboratory — Geometric frustration in Mott insulators permits perturbative electron fluctuations controlled by local spin configurations [1]. An equilateral triangle ("trimer") of spins with S = 1/2 is the simplest example, in which low-energy degrees of freedom consist of built-in magnetic and electric dipoles arising from the frustrated exchange interaction. Such trimers can be weakly coupled to make multiferroics by design [2]. An organic molecular magnet known as TNN, with three S = 1/2 nitronyl nitroxide radicals in a perfect C_3 symmetric arrangement, is an ideal building block as demonstrated by recent experiments on a single crystal comprising TNN and CH_3CN. The fascinating thermodynamic phase diagram of this molecular crystal, TNN•CH_3CN, is in excellent agreement with our theory, which predicts multiferroic behavior and strong magnetoelectric effects arising from an interplay between magnetic and orbital degrees of freedom. Our study thus opens up new avenues for designing multiferroic materials using frustrated molecular magnets. References: [1] L. N. Bulaevskii *et al.*, PRB **78**, 024402 (2008). [2] Y. Kamiya and C. D. Batista, PRL **108**, 097202 (2012).

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