Multiferroics by design: how to build multiferroic materials with a frustrated molecular magnet

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Geometrical frustration refers to a lattice system whose ground state cannot satisfy all the interactions simultaneously, quite often arising from antiferromagnetic triangular motifs. Frustrated magnets can have a low-energy manifold of nearly degenerate states from which interesting phenomena may emerge, such as exotic magnetic and nonmagnetic orders, topological order, liquid-like or even glassy behavior, and so on, varying from one material to another. Furthermore, geometrical frustration enables the interplay between local magnetic and electric dipole moments in a strongly correlated Mott insulator [1, 2]. The simplest example would be a molecular magnet with three spin-1/2 moments forming an equilateral triangle, where the low-energy states possess built-in magnetic and electric dipoles arising from the frustrated exchange interaction. We discuss that the trimers can then be used as building blocks for constructing multiferroics by design. By starting from an organic quantum spin trimer, known as TNN, as the elementary unit, the triangular trimer crystal TNN•CH_3CN was synthesized some years ago, which was shown to exhibit strong magneto-electric effects [3]. We show that the measured thermodynamic phase diagram is in excellent agreement with our theory, revealing exotic behaviors out of the interplay between magnetic and intra-trimer orbital degrees of freedom [4]. We hope that our study has opened a new avenue for designing multiferroic materials with frustrated molecular magnets.
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