MS24-01 | A Symmetry Motivated Approach for Enumerating Magnetoelectric Couplings in Perovskites

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A group-theoretical approach is used to enumerate the possible couplings between magnetism and ferroelectric polarization in the parent Pm-3m perovskite structure. It is shown that third-order magnetoelectric coupling terms must always involve magnetic ordering at the A and B sites which either transforms both as R-point or both as X-point time-odd irreducible representations (irreps). For fourth-order couplings it is demonstrated that this criterion may be relaxed allowing couplings involving irreps at X-, M- and R-points which collectively conserve crystal momentum, producing a magnetoelectric effect arising from only B-site magnetic order. In this case, exactly two of the three irreps entering the order parameter must be time-odd irreps and either one or all must be odd with respect to inversion symmetry. It is possible to show that the time-even irreps in this triad must transform as one of: X_1^+, $M_{3,5}^-$ or R_5^+, corresponding to A-site cation order, A-site antipolar displacements or anion rocksalt ordering, respectively. This greatly reduces the search space for type-II multiferroic perovskites. Similar arguments are used to demonstrate how weak ferromagnetism may be engineered and a variety of schemes are proposed for coupling this to ferroelectric polarization. By considering the literature, suggestions are given of which avenues of research are likely to be most promising in the design of novel magnetoelectric materials.