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The search for new multiferroic ABF_4 fluorides via first-principles structure maps BRIAN ABBETT, ADITI KRISHNAPRIYAN[1], CRAIG J. FENNIE, Cornell University — Transition metal ABF_4 fluorides are observed in a wide variety of different structure types. One, the $BaMnF_4$ structure, is an interesting family of polar (possibly ferroelectric) materials that display canted-antiferromagnetism, which has been predicted (Ederer and Spaldin) to reverse when the polarization reverses. This strong coupling between magnetism and polarization has motivated us to explore additional ABF_4 structure types. In this talk we will discuss our search for new multiferroic ABF_4 fluorides by creating structure maps from first principles. As a first step we categorize the ABF_4 compounds found in the ICSD. We focus on structures for which the B-site is octahedrally coordinated; these can be fitted into one of four categories: $BaMF_4$, Dion-Jacobson, and the so-called slip (100) or slip (110) structures. These four categories represent high symmetry structures which allow distortions to lower symmetry structures. Note that most of the known multiferroic ABF_4 compounds form in the $BaMF_4$ structure. We elucidate a simple descriptor that helps to build the chemical and physical intuition as to why a compound forms in this structure type needed for the rational design of new multiferroic ABF_4 fluorides.

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