High-throughput database search of antiferroelectric materials in ABX_2

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We use a first-principles rational design approach to identify a previously unrecognized class of antiferroelectric materials in the ABX_2 family of compounds. We perform a high-throughput scan of a large number of ABX_2 compounds in the ICSD[1] database, testing for dielectric and structural conditions leading to antiferroelectricity. The *Pnma* $SrCN_2$ structure type can be described in terms of antipolar distortions of the nonpolar *Immm* $NaNO_2$ structure type, present in the ferroelectric compound $NaNO_2$. We find members of the *Pnma* $SrCN_2$ structure type close in energy to the related polar *Imm2* $NaNO_2$ structure type, which includes members we predict to be ferroelectric. We calculate structural parameters and relative energies for all three structure types, both for reported and hypothetical representatives of this class. Our results provide guidance for experimental realizations and further investigation of high-performance materials suitable for practical applications.

[1] A. Belsky, M. Hellenbrandt, V. L. Karen, and P. Luksch, Acta Crystallogr. Sect. B **58**, 364 (2002).