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**Why are there so few perovskite ferroelectrics?** NICOLE BENEDEK, The University of Texas at Austin, CRAIG FENNIE, Cornell University — Nearly all cubic $ABO_3$ perovskites are unstable to energy-lowering structural distortions, the most common being those that give rise to ferroelectricity (usually an off-centering of the B-site cation) and tilts or rotations of the $BO_6$ octahedra. Whereas there are many perovskites that are either ferroelectric or have rotated octahedra, there are very few perovskites that are both ferroelectric and have rotated octahedra. This observation has lead to the widespread assumption that rotations suppress ferroelectricity and vice versa. Using first-principles density functional theory calculations, in combination with crystal chemistry and symmetry principles, we show that rotations do not always suppress ferroelectricity. In fact, the most fertile place to search for new ferroelectrics may be the place that has thus far been considered the least likely to contain them: materials that are expected to have large rotations. We will show why and how ferroelectricity is suppressed in the most common space group adopted by perovskites (Pnma) and explain how we can use this knowledge to design new ferroelectrics and functional materials.

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