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Competition and cooperation between octahedral rotations and ferroelectricity in simple and layered ABX_3 perovskites

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Researchers have been studying octahedral rotations in perovskites for over half a century. It is now known that such lattice distortions are generally driven by the coordination preferences of the A-site cation. The role of octahedral rotations in modulating the magnetic, electronic and orbital properties of perovskites has been elucidated and a set of empirical rules for rationalizing the structures of known materials and for predicting the structures of as yet unsynthesized materials has been established. Despite this progress, there remains a long-standing problem concerning octahedral rotations and ferroelectricity: there are very few ferroelectric ABX_3 perovskites with octahedral rotations. This has lead to the widespread assumption that octahedral rotations compete with and suppress ferroelectricity. In this talk, I will describe our recent work on the interaction between ferroelectricity and octahedral rotations in simple and layered perovskites. Using a combination of Density Functional Theory and simple crystal chemical models, we have shown that in contrast to the common assumption, ferroelectricity and octahedral rotations do not always compete. In particular, I will discuss the manner in which rotations can actually induce ferroelectricity in ABX_3 perovskites and present strategies for designing new functional materials based on this mechanism. In a related direction, I will also discuss the role of layering in inducing hybrid improper ferroelectricity in some Ruddlesden-Popper phases and double perovskites. Our approach provides a chemically intuitive picture – one that combines first-principles lattice dynamics with a local description of bonding – to explain why particular materials adopt particular structures. Such knowledge is at the foundation of the current materials-by-design effort.