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Turning ABO_3 antiferroelectrics into ferroelectrics: Design rules for practical rotation-driven ferroelectricity in double perovskites and Ruddlesden-Popper compounds ANDREW T. MULDER, School of Applied and Engineering Physics, Cornell University, NICOLE A. BENEDEK, Materials Science and Engineering Program, The University of Texas at Austin, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, CRAIG J. FENNIE, School of Applied & Engineering Physics, Cornell University — The discovery of octahedral rotation-induced ferroelectricity has provided a new avenue to realize novel materials to explore the interplay of the electrical polarization and correlated phenomena such as magnetism. Design rules recently established suggest ferroelectricity will exist in layered $AA'B_2O_6$ perovskites when at least one of the ABO_3 constituents forms in the nonpolar Pnma structure. As the majority of perovskites form in Pnma, these rules are widely accessible to many chemistries and therefore have the potential to lead to new classes of multifunctional materials. This recent advance however does not directly address the question of whether or not this polar state is a functional ferroelectric or simply a pyroelectric. In this talk we derive from first principles a chemically and physically intuitive model, based only on the properties of the ABO_3 constituents, to guide the realization of both large polarizations and small ferroelectric switching barriers. We show how this model follows from a complex interplay of octahedral rotations, antiferroelectric lattice distortions inherent in every Pnma material, and A-site cation ordering. Finally we demonstrate its applicability not only to the double perovskites but also to Ruddlesden-Popper compounds.

Andrew T. Mulder
School of Applied and Engineering Physics, Cornell University

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