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Crossover between hybrid improper ferroelectricity and proper ferroelectricity in layered perovskites ANDREW MULDER, NICOLE BENEDEK, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University — Recent progress in designing materials with unconventional mechanisms of ferroelectricity has shown that nominally non-polar octahedral rotations can induce an electrical polarization in certain layered perovskites, e.g., the $n=2$ Ruddlesden-Popper $\text{Ca}_3\text{Mn}_2\text{O}_7$, and certain A-site ordered $\text{AA}'\text{B}_2\text{O}_6$ double perovskites. In these (what have recently been termed) hybrid improper ferroelectrics, two unstable octahedral rotations of different symmetries couple trilinearly with the polarization. A key question that is still unclear is what the consequences of this coupling are in determining whether these materials exhibit conventional proper ferroelectricity, as in $\text{SrBi}_2\text{Ta}_2\text{O}_9$, or something resembling improper ferroelectricity. In this talk we discuss this question of proper vs improper in $\text{A}_3\text{B}_2\text{O}_7$ layered perovskites. First we develop simple criteria for realizing this novel form of ferroelectricity based solely on the properties of the ABO_3 parent perovskites. Then we explore how composition and epitaxial strain lead to different ferroelectric behaviors arising from the same rotation-polarization coupling. Finally we show how strain can tune a single material between rotation-driven hybrid improper ferroelectricity and conventional proper ferroelectricity.

Andrew Mulder
School of Applied and Engineering Physics, Cornell University

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