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**Potential Hybrid Improper Ferroelectricity in the Oxyfluoride  $\text{KNaNbOF}_5$**  JAYE HARADA, Northwestern University, NENIAN CHARLES, Drexel University, JUAN NINO, University of Florida, KENNETH POEPELMEIER, JAMES RONDINELLI, Northwestern University — We assess whether the observed displacive transition between a low temperature polar and high temperature centrosymmetric phase of the oxyfluoride  $\text{KNaNbOF}_5$  is proper or improper using a combination of materials theory and experimentation. Although the transition appears to occur at a single critical temperature, crystallographic mode analyses shows that two lattice modes are required to produce the structure of the low-symmetry phase; these facts together suggest an improper character requiring further investigation. First, we experimentally verify the order of the transition using dielectric measurements and differential scanning calorimetry. Then, using density functional theory calculations and phenomenological Landau theory, we determine the relevance of permitted trilinear multimode interactions on the stability of the observed ground state and the suppression of potential intermediate phases. Based on these simulations, we also discuss the potential for experimental switching of the ferroelectric polarization.

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