

Abstract Submitted
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Strain-Induced Geometric Ferroelectricity in Perovskite-structured Fluoroscandates NENIAN CHARLES, Drexel University, JAMES RONDINELLI, Northwestern University — Using first-principles density functional theory calculations we investigate geometric ferroelectricity in epitaxially strained double-perovskite fluorides, Na_3ScF_6 and K_2NaScF_6 . The experimental room temperature crystal structures of the fluoroscandates are centrosymmetric, i.e. Na_3ScF_6 ($P2_1/n$) and K_2NaScF_6 ($Fm\bar{3}m$). However, in their prototypical cubic geometry, we identify soft infrared active modes that are strongly sensitive to pressure: Ferroelectric instabilities are found for negative hydrostatic pressures ~ -6 GPa. For Na_3ScF_6 we observe octahedral rotations ($a^-a^-c^+$ tilt system) are in strong competition with acentric polar distortions, and as a result exceedingly large tensile strain above 8% are required to stabilize a Pm polar phase. We demonstrate that the strain mismatch required to stabilize the ferroelectric phase can be reduced to approximately 4% with chemical substitution in $(a^0a^0a^0)$ K_2NaScF_6 by reducing the tendency to octahedral rotations. Our study provides new insights that may prove useful in guiding experimental efforts towards identifying functional polar fluoroperovskites.

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