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A-site driven ferroelectricity in $\mathbf{K_{0.5}Li_{0.5}NbO_3}$ DANIEL I. BILC, D.J. SINGH, Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Mixed A-site ferroelectric materials have gained recent attention. Here we report density functional calculations of $K_xLi_{1-x}NbO_3$ perovskite supercells in order to understand the interplay between various lattice instabilities with size mismatch on the A-site and the role of the A and B site ions in this case. The calculations were done using the general potential LAPW method. For x=0.5, we find a ferroelectric ground state, even though the average tolerance factor is significantly smaller than unity and there is no stereochemically active A site ion. This is due to frustration due to the very different ionic radii of K and Li. We find very large off-centering of the Li ions, which distinguishes this compound. Relative to this the Nb off-centering is quite small. This is in contrast to most perovskite ferroelectrics where there is significant off-centering of all ions, and resulting cooperativity. Also because of the large Li off-centering it contributes strongly to the anisotropy between tetragonal and rhombohedral ground states, yielding a tetragonal ground state. Normally the anisotropy is determined by the interplay of B site off-centering and strain coupling. This work was supported by the Office of Naval Research and the Department of Energy.

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