A-site driven ferroelectricity in 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$_x$Li$_{1-x}$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.

Daniel Bilc
Condensed Matter Sciences Division, Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Date submitted: 23 Nov 2005

Electronic form version 1.4