

Design of novel ferroelectric materials via compositional inversion symmetry breaking

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Using ultrasoft-pseudopotential calculations within the local density approximation we have studied cubic perovskite compounds of the form $(A_{1/3}A'_{1/3}A''_{1/3})BO_3$ and $A(B_{1/3}B'_{1/3}B''_{1/3})O_3$, in which three different cations on the A or B sublattice form alternating series of monolayers along the (001) direction. It has been proposed [1] that such materials may be grown by molecular epitaxy. These compounds will be representatives of a possible new class of materials in which ferroelectricity is perturbed by compositional breaking of the inversion symmetry.

For isovalent substitution on either sublattice, the ferroelectric double-well potential is found to persist, but becomes sufficiently asymmetric that minority domains may no longer survive. The strength of the symmetry breaking is enormously stronger for heterovalent substitution, so that the double-well behavior is completely destroyed. We will show that by varying the layer-by-layer composition it is possible to tune systems continuously between these two behaviors, which may allow to optimize a desired characteristic of the material, such as, for example, the piezoelectric response.

[1] Jim Eckstein, privat communication