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Energy-polarization behaviors of $AA'BB'O_6$ perovskites with double rock-salt order ANINDYA ROY, DAVID VANDERBILT, Rutgers University — Using first-principles methods, we study the energy-polarization relation of double perovskites $AA'BB'O_6$ where atoms in both A and B sites are arranged in rock-salt order. The high-symmetry structure in this case is the *tetrahedral* $F\bar{4}3m$ space group. If a ferroelectric instability occurs, the energy-vs.-polarization landscape $E(\mathbf{P})$ will tend to have minima for $\mathbf{P}$ along tetrahedral directions leading to a rhombohedral space group $R3m$, with two different values of spontaneous polarization and associated energy along opposite body-diagonal directions; or along Cartesian directions, leading to orthorhombic space group $Imm2$. We search for polar *soft modes* at the Γ point of the high-symmetry $F\bar{4}3m$ structure and analyze its eigenvectors to identify ferroelectric instabilities, which we find in $CaBaTiZrO_6$, $KCaZrNbO_6$ and $PbSnTiZrO_6$. The results of the first-principle calculations are modeled with a Landau-Devonshire expansion that is truncated at either 4th or 5th order in $\mathbf{P}$, and its predictions are found to agree favorably with our calculation. The 5th-order calculation improves the agreement further except in PSTZ. Recently, synthesis of $SrCaTiMnO_6$ in rock-salt order has been reported.[1] Unfortunately, preliminary results do not seem to indicate any polarized structure.

[1]J.L Blok, G. Rijnders and D.H.A. Blank, private communication.

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