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Polar Behavior of Double Perovskites $BiPbZnNbO_6$ and $BiSrZnNbO_6$: A First Principles Study[1] SHIGEYUKI TAKAGI, ALASKA SUBEDI, Materials Science and Technology Division, Oak Ridge National Laboratory, Department of Physics, University of Tennessee, DAVID J. SINGH, VALENTINO R. COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory — Perovskites are classed in two groups, A- and B-site driven materials, according to the tolerance factor t. In the majority of A-site driven materials, which have $t < 1$, BO_6 octahedra are tilted and they are not ferroelectrics except for perovskite with lone-pair A-sites such as Pb and Bi. However, if the octahedra are prevented from tilting by mixing large and small A-site ions, they may become strong ferroelectrics. Here we report the polar behavior of $BiPbZnNbO_6$ and $BiSrZnNbO_6$ based on first principles supercell calculation. The motivation of these choices come from the ion size differences of Pb and Sr as compared with Bi. Additionally, while Pb and Sr ions have approximately the same size, Pb has a low lying $6p$ state. An anomalously large Z^* are found on the Pb compared with one on Sr. It implies there is stronger covalency of Pb-O than one of Sr-O reflecting the absence of $6p$ state on Sr. The polarizations were $\sim 40 \mu C/cm^2$. These perovskites, especially Pb, will be good candidates for new ferroelectric materials.

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