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Effect of A-site size difference on polar behavior in MBiScNbO$_6$ (M=Na, K, and Rb) perovskite: Density functional calculations SHIGEYUKI TAKAGI, ALASKA SUBEDI, Oak Ridge National Laboratory and University of Tennessee, VALENTINO COOPER, DAVID SINGH, Oak Ridge National Laboratory — We investigated the effect of A-site size difference in the double perovskites $BiScO_3$-$MNbO_3$ (M=Na, K, and Rb) using first-principles calculations. The materials studied have increasing ionic radii at the A-site ($r_{Na^+} < r_{K^+} < r_{Rb^+}$) but are otherwise chemically similar. We find that the polarization of these materials is 70-90 $\mu C/cm^2$ along the rhombohedral direction, which increases as the A-site size difference becomes larger. The main contribution to the high polarization comes from large off-centerings of Bi ions, which are strongly enhanced by the suppression of octahedral tilts as the M-ion size increases. A high Born effective charge of Nb also contributes to the polarization and this contribution is also enhanced by increasing the M-ion size. This work was supported by ONR and DOE, BES, Materials Sciences and Engineering.

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