Ferroelectric properties in PbZrO$_3$/BaZrO$_3$ superlattices: an ab-initio study

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University of Nebraska at Omaha — Properties of tetragonal (BaZrO$_3$)$_n$/(PbZrO$_3$)$_n$ ferroelectric superlattices with $n = 1$–3 are calculated from first principles within the density functional theory. We show that an antiferroelectric PbZrO$_3$ displays ferroelectric behavior if deposited on a paraelectric substrate (BaZrO$_3$). We have performed total energy calculations to investigate the origins of the ferroelectricity and analyze the polarization of BaZrO$_3$/(PbZrO$_3$)$_n$ superlattices as function of PbZrO$_3$ thickness. The densities of states (DOS) show that there is a strong hybridization between Zr/Pb and O atoms which play important role in stabilizing the ferroelectric ground state in the superlattices. Our calculations show that the polarization and tetragonality ($c/a$ ratio) are reduced in the BaZrO$_3$/PbZrO$_3$ superlattices with respect to bulk tetragonal PbZrO$_3$. Moreover, the tetragonality and polarizations of superlattices increase with increasing the fraction of PbZrO$_3$ in the superlattices. The estimated polarization of the (BaZrO$_3$)$_1$/(PbZrO$_3$)$_1$ superlattice is $(38.46 \mu C/cm^2)$, while it is $(56.82 \mu C/cm^2)$ for the (BaZrO$_3$)$_1$/(PbZrO$_3$)$_3$ superlattice and $(74.22 \mu C/cm^2)$ for bulk tetragonal PbZrO$_3$. These ferroelectric superlattices have good lattice matching with shape-memory NiMnIn Heusler alloys and could be very useful as a ferroelectric substrate to systems.

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