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Ferroelectric properties in $PbZrO_3/BaZrO_3$ superlattices: an *ab-initio* study NABIL AL-AQTASH, AHMAD ALSAAD, RENAT SABIRIANOV, University of Nebraska at Omaha — Properties of tetragonal $(BaZrO_3)_1/(PbZrO_3)_n$ 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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