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Theoretical prediction of new high-performance lead-free ferroelectrics PIO BAETTIG, CHARLES SCHELLE, NICOLA SPALDIN, Materials Department UCSB Santa Barbara, RICHARD LESAR, LANL Los Alamos, UMESH WAGHMARE, J. Nehru Centre for Advanced Scientific Research, Bangalore, India
— We predict the occurence of large ferroelectric polarization and piezoelectricity in the hypothetical perovskite-structure oxides, bismuth aluminate ($BiAlO_3$) and bismuth gallate ($BiGaO_3$), using density functional theory within the local density approximation. We show that $BiGaO_3$ will have a similar structure to $PbTiO_3$, although with much stronger tetragonal distortion and therefore improved ferroelectric properties. Likewise, $BiAlO_3$ shares structural characteristics with antiferrodistortive $PbZrO_3$, but it is also a ferroelectric with large polarization. Therefore we propose the $Bi(Al,Ga)O_3$ system as a replacement for the widely used piezoelectric sensor, $Pb(Zr,Ti)O_3$ (PZT) that will avoid the environmental toxicity problems of lead-based compounds. Finally we show that, in both $BiAlO_3$ and $BiGaO_3$, the large distortions from the prototypical cubic structure are driven by the stereochemical activity of the Bi lone pair.

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