Electric-field switching of polar displacements in a newly predicted polar metal

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Polar metals--analogy of ferroelectrics in metals--are characterized by intrinsic conduction and inversion symmetry breaking. Polar metals are rare (especially in oxides) because mobile electrons screen electric fields in a metal and eliminate internal dipoles that are needed to break inversion symmetry. The discovery of $LiOsO_3$ [1], a metal that transforms from a centrosymmetric *R-3c* structure to a polar *R3c* structure at 140 K, has stimulated an active search for new polar metals in both theory and experiment.

In our study [2], we combine first-principles calculations and crystal structure search method to predict a new polar metal and demonstrate 180° electric-field switching of its polar displacements. Utilizing lone-pair electrons and different valences of Bi and Pb, ordered $BiPbTi_2O_6$ can crystallize in three polar and conducting structures, each of which can be transformed to another via pressure or strain. In a heterostructure of layered $BiPbTi_2O_6$ and $PbTiO_3$, a strong interfacial coupling enables electric fields to first switch $PbTiO_3$ polarization and subsequently drive a 180° change of $BiPbTi_2O_6$ polar displacements. Our work demonstrates the power of high-throughput screening in designing new functional materials and in particular predicts a new electrically switchable polar metal.

References:

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