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Control of octahedral rotations for the design of largely enhanced ferroelectricity and related functionalities in perovskites

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Ferroelectric polarization in perovskite materials is closely associated with the pattern of its oxygen octahedral rotations, which are common structural distortions in perovskites. The oxygen rotation pattern in $BiFeO_3$ with R3C symmetry promotes large electric polarization. On the contrary, oxygen rotation pattern in $CaTiO_3$ of Pbnm symmetry strongly suppresses the ferroelectricity. For many $CaTiO_3$ -like perovskites, the $BiFeO_3$ -like structure is a metastable phase. Our Landau phenomenological theory reveals that the stability of either a $CaTiO_3$ -like or a $BiFeO_3$ -like structure in perovskite is sensitively dependent on the structural distortions, which could be effectively adjusted by material engineering approaches and external stimulus. Here, we report the stabilization of the highly-polar $BiFeO_3$ -like phase in nonpolar orthorhombic perovskites based on interface engineering, epitaxial strain, applied electric fields etc. Our results suggest that a large number of perovskites with the $CaTiO_3$ structure type, which include many magnetic representatives, are now good candidates as novel highly-polar multiferroic materials.